

Developing Strategies for the Reduction of Greenhouse Gas Emissions from Wastewater Treatment

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as a thesis for the degree of
Doctor of Philosophy in Engineering
In October 2014

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ABSTRACT

This thesis investigates the potential of improved control to reduce greenhouse gas (GHG) emissions resulting from existing wastewater treatment plants (WWTPs), and demonstrates that significant reductions can be achieved without the need for extensive redesign of treatment processes and without increasing operational costs.

An emissions model is developed for use in this study, informed by an in-depth analysis of existing state-of-the-art methods and models for estimating GHG emissions, taking into account their suitability for dynamic modelling and WWTP control strategy optimisation. Through the use of local and global sensitivity analysis tools, sources of uncertainty in the modelling of GHG emissions from wastewater treatment are investigated, revealing critical parameters and parameter interactions; these interaction effects have not been considered in previous studies and thus provide a better understanding of WWTP model characterisation. A key finding is that uncertainty in modelled nitrous oxide (N_2O) emissions is the primary contributor to uncertainty in total GHG emissions, due largely to the interaction effects of nitrogen conversion modelling parameters.

Further local and global sensitivity analysis is used to investigate the effects of adjusting control handle values on GHG emissions, revealing critical control handles and sensitive emission sources for control. This knowledge assists with the following control strategy development and aids an efficient design and optimisation process. Sources with the greatest variance in emissions, and therefore the greatest need to monitor, are also identified. It is found that variance in total emissions is predominantly due to changes in direct N_2O emissions and selection of suitable values for wastage flow rate and aeration intensity in the final activated sludge reactor is of key importance.

Sets of Pareto optimal operational and control parameter values are derived using a multi-objective genetic algorithm, NSGA-II, with objectives including minimisation of GHG emissions, operational costs and effluent pollutant concentrations, subject to legislative compliance. It is found that multi-objective optimisation can facilitate a significant reduction in GHG emissions without the need for plant redesign or modification of the control strategy layout, but there

are trade-offs to consider: most importantly, if operational costs are not to be increased, reduction of GHG emissions is likely to incur an increase in effluent ammonia and total nitrogen concentrations. Alternative control strategies are also investigated and it is concluded that independent control of dissolved oxygen in each aerated activated sludge reactor is beneficial.

Optimised solutions are also assessed with respect to their reliability, robustness and resilience, taking into account the effects of influent perturbations and sensor failures on effluent quality and GHG emissions. This reveals that solutions predicted to achieve the most significant reductions in GHG emissions and operational costs under existing design conditions may perform poorly in reality when subject to threats. Dissolved oxygen setpoints which correspond with unacceptable effluent quality reliability and decision variables which should not be considered in future optimisation due to their negative impacts on reliability, robustness and resilience are also identified.

Lastly, guidelines for the development of control strategies to reduce GHG emissions are presented. These address GHG emission sources, key control handles and decision variables, choice of control strategy, optimisation and detailed design, and model limitations and uncertainties.

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ACKNOWLEDGEMENTS

I would like to express my gratitude to my supervisors, Professor David Butler and Dr Guangtao Fu, whose guidance, expertise and encouragement throughout my studies have been invaluable. I would also like to thank all the staff and students in the Centre for Water Systems, both past and present, with whom I have had the pleasure of working. Their knowledge and enthusiasm has been inspirational and their friendship has made the overall PhD experience much more enjoyable.

I am also appreciative of everyone outside the University that I have been in contact with and who has provided assistance – be that technical guidance, provision of information, site visits or other forms of support. Particular thanks are due to Jules Florey of South West Water for time she gave me and for supplying data (albeit for a case study site that was eventually deemed unsuitable and not used).

I gratefully acknowledge financial support provided by the University of Exeter in the form of a studentship. Thanks are also given for the Matlab/Simulink implementation of the BSM2 from the Department of Industrial Electrical Engineering and Automation, Lund University, Lund, Sweden, and for David Hadka's C++ code for implementation of Sobol's sensitivity analysis.

Last, but by no means least, I would like to thank all my friends and family who have put up with and supported me for the last three years – in particular Adrian, Fiona and Elaine.

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LIST OF ABBREVIATIONS

ADM1	Anaerobic Digestion Model No. 1
AOB	Ammonium-oxidising bacteria
ASCE	American Society of Civil Engineers
ASM1	Activated Sludge Model No. 1
ASM2d	Activated Sludge Model No. 2d
ASMG1	Activated Sludge Model for Greenhouse Gases No. 1
ASMG2d	Activated Sludge Model for Greenhouse Gases No. 2d
ASMN	Activated Sludge Model for Nitrogen
BOD	Biochemical oxygen demand
BOD _u	Ultimate BOD
BSM2	Benchmark Simulation Model No. 2
BSM2G	Benchmark Simulation Model No. 2 for Greenhouse Gases
CH ₄	Methane
CHPA	Combined Heat & Power Association
CL	Closed loop
CO ₂	Carbon dioxide
CO _{2e}	Carbon dioxide equivalent
COD	Chemical oxygen demand
CRC	Carbon Reduction Commitment
DECC	Department of Energy & Climate Change
DO	Dissolved oxygen
DOL	Default open loop
EF	Emission factor

GHG	Greenhouse gas
GSA	Global sensitivity analysis
GWP	Global warming potential
HRT	Hydraulic residence time
HSC	Half saturation coefficient
IPCC	Intergovernmental Panel on Climate Change
IWA	International Water Association
LCA	Life cycle assessment
N ₂ O	Nitrous oxide
OAT	One-factor-at-a-time
OL	Open loop
PE	Population equivalent
PI	Proportional integral
SRT	Solids retention time
TSS	Total suspended solids
UKWIR	UK Water Industry Research
USEPA	U.S. Environmental Protection Agency
UWWTD	Urban Waste Water Treatment Directive
VSS	Volatile suspended solids
WEF	Water Environment Federation
WFD	Water Framework Directive
WWTP	Wastewater treatment plant

1 INTRODUCTION AND SCOPE

1.1 Background

Developing strategies for the reduction of greenhouse gas (GHG) emissions is a topic of great interest and current relevance, as global warming is an internationally recognised problem. To help address this, the UK has committed to reduce its GHG emissions by 20% by 2020 and at least 80% by 2050 compared with respect to a 1990 baseline, under the Climate Change Act 2008. Other countries have also committed to emission reduction targets under the Kyoto Protocol to mitigate the effects of global warming.

Recent studies have highlighted the significance of GHG emissions resulting from energy use in the water industry (e.g. Rothausen and Conway 2011); whilst in Europe it only typically contributes 1% of national consumption, this is predicted to increase (Olsson 2012), and in the U.S.A. 4% of electricity demand is attributable to the movement and treatment of water and wastewater (Mo et al. 2010). As such, the water industry must contribute to the 80% emission target, using a range of mitigation and adaptation strategies.

Reduction of emissions from wastewater treatment is a high priority, as it is attributed with producing 56% of the water industry's emissions associated with energy use (Defra 2008). Wastewater treatment also results in the formation and direct emission of the GHGs carbon dioxide (CO₂), methane (CH₄) and nitrous oxide (N₂O), as well as indirect emissions resulting from chemical manufacture and sludge disposal, amongst other sources. The wastewater sector was responsible for over 5% of global non-CO₂ GHG emissions in 2005, and these emissions are predicted to increase by 27% (i.e. to over 6% of global non-CO₂ GHG emissions) by 2030 (U.S. Environmental Protection Agency 2012).

The demands on emission reduction must be met whilst also complying with increased water quality standards required by the Water Framework Directive, which has the potential to increase annual CO₂ emissions by more than 5% if there is no intervention, due to operational energy use and additional processes required (derived from Defra 2008, Georges et al. 2009), and provides no incentives for investment in low carbon solutions. The water industry is, therefore, faced with the huge challenge of reducing carbon emissions by 80%

whilst improving standards and remaining cost efficient. Further challenge is posed by the knowledge that reducing energy consumption does not necessarily correspond to a reduction in GHG emissions and local energy optimisation can, in fact, increase the total global warming potential of emissions from a wastewater treatment plant (WWTP) (Flores-Alsina et al. 2014).

It is recognised that appropriate design and operation of wastewater treatment processes can play a significant role in mitigating the effects of global warming (Gori et al. 2011) and it is thought that significant emission reductions could be achieved by optimising existing processes. However, whilst there has been significant research into the optimisation of WWTP management strategies to increase efficiency, few attempts at optimisation have been made with the objective of minimising GHG emissions.

1.2 Definition and Quantification of Greenhouse Gases

GHGs are gases which absorb and emit thermal infrared radiation from the Earth's surface, clouds and the atmosphere (IPCC 2007), leading to a greenhouse effect as they absorb energy that would otherwise leave the Earth's atmosphere. Without GHGs, the equilibrium temperature of the Earth would be reduced, as less infrared radiation would be absorbed. However the increasing concentration of GHGs in the atmosphere during the industrial era is widely believed to be the most contributing factor in rising global temperatures. As such, increasing efforts are being made to reduce GHGs and limit the effects of global warming.

Examples of GHGs include CO₂, CH₄, N₂O, halocarbons, ozone, water vapour and aerosols. Several (e.g. CO₂ and CH₄) occur naturally but are also emitted as a result of human activity. However others, such as fluorinated gases, are only synthesised and emitted as a result of human activity (EPA 2014).

The contribution of each individual GHG to the greenhouse effect is dependent on its molecular characteristics in addition to its concentration in the atmosphere. For example the effects of a N₂O molecule are 310 times greater than those of a CO₂ molecule for a 100 year time horizon, and a CH₄ molecule 21 times greater (Forester et al. 2007). When analysing systems which emit more than one GHG, a framework is required to determine the trade-off

between different emission compositions and enable the development of mitigation measures in a decentralised manner. A simple method is to use a Global Warming Potential (GWP) index to define the contribution of every GHG to climate change over a set time period with respect to that of an equivalent mass of CO₂. This concept enables mixed emissions to be expressed in terms of carbon dioxide equivalent (CO₂e), where the CO₂e of each gas is the product of its mass and 100 year GWP. Whilst the adequacy of GWPs has been questioned due to the simplifications involved, it has been adopted for use in the Kyoto Protocol and is widely used for quantification of GHG emissions.

1.2.1 Legislative Constraints and Drivers for Change

Carbon Reduction Commitment

The Carbon Reduction Commitment (CRC) Energy Efficiency Scheme was introduced by the UK government in 2008 to deal with carbon emissions that are not already covered by the EU Emissions Trading Scheme or Climate Change Agreements, and to help the country meet its target under the Kyoto Protocol of reducing GHG emission by 80% by 2050 with respect to a 1990 baseline. The scheme came into operation in April 2010 and all organisations which consumed at least 6,000 MWh of electricity (approximately £500,000 worth) during the qualification year are legally compelled to participate (DECC 2014). By employing a range of drivers, it aims to significantly improve efficiency and cut emissions from all large private and public sector organisations.

As a result of the CRC, water companies are obliged to measure and report their annual carbon emissions from energy supplies, using specified conversion factors for different energy sources. These emissions calculations are used in production of the compulsory 'footprint report' and 'annual report'. Initially, following the submission of these reports, performance league tables ranking the relative performance of each participant were published; however, this has now been replaced with an annual report containing aggregated emissions data for all participants.

As of 2012, participating companies are required to purchase and surrender CRC allowances from the government each year to offset their emissions. For 2014-15, these allowances may be bought in advance at a cost of £15.60 per

tonne of CO₂, based on predicted emissions, and additional allowances required for compliance at the end of the period purchased at an increased price of £16.40 per tonne of CO₂ (CHPA 2013).

Urban Wastewater Treatment Directive

The collection and treatment of urban wastewater in England and Wales is controlled by the Urban Waste Water Treatment (England and Wales) Regulations 1994, in accordance with the EU Urban Waste Water Treatment Directive (UWWTD) (91/271/EEC). These regulations specify minimum treatment levels based on the size of the discharge and the sensitivity of the receiving water body, and state that all urban areas above 2,000 population equivalent must have a sewerage system, from which collected sewage must receive at least secondary treatment before it is discharged. More stringent standards are given to discharges into sensitive areas and untreated discharges are only allowed under storm conditions.

Water Framework Directive

The European Water Framework Directive (WFD) (2000/60/EC) was developed to replace a range of existing European legislation relating to the protection of rivers, lakes, groundwaters, estuaries and seas, and to provide a more consistent, integrated approach to the management of water bodies throughout Europe. The primary objective of the WFD is to achieve a 'good ecological status' and a 'good chemical status' for all surface waters by 2015. Whilst it specifies biological elements which must contribute to the ecological status, development of a suitable assessment system and definition of a 'good' status is the responsibility of individual Member States.

The WFD came into force in December 2000 and was transposed into UK domestic law through the following regulations:

- The Water Environment (Water Framework Directive) (England and Wales) Regulations 2003
- The Water Environment and Water Services (Scotland) Act 2003
- The Water Framework Directive (Implementation) Regulations (Northern Ireland) 2003

Additional regulations cover cross border (England/Scotland) river basin districts. For each river basin district, a complete analysis of the surface and groundwater characteristics, a review of the environmental impact of human activity and an economic analysis of water use were undertaken, and monitoring programmes and work programmes were later introduced to counter any upward trends in pollution identified. River basin management plans, including environmental objectives for each body of surface or groundwater, were published in 2009 and an implementation report published in 2012, in which WWTPs were identified as one of the greatest contributors to chemical pollution (European Commission 2012).

1.2.2 Strategies for Emission Reduction

Strategies for the reduction of GHG emissions resulting from wastewater treatment whilst meeting the WFD obligations could include the following: increased operational efficiencies, renewable energy generation and change of operational procedures (Georges et al. 2009). Further information on how use of each could contribute to a reduction in overall emissions is given in the following sections. Additional options identified (Georges et al. 2009) include source control and least-carbon end of pipe / process addition (i.e. acceptance that an increase in emissions is inevitable and finding the least-carbon solution), and redevelopment of existing treatment processes. Source control is likely to bring significant savings, but the water industry has limited power to achieve this. Redevelopment of existing treatment processes is beyond the scope of this research, since it aims to investigate the potential for emission reduction from existing WWTPs by improved operation and control alone, which may encompass increased operational efficiencies and increased generation of renewable energy.

Increased Operational Efficiencies

Whilst some plants modify schedules for equipment operation in reaction to changing load conditions during the course of a day, others operate them at full capacity continuously, regardless of the load (Metcalf and Eddy 1994) (although this is increasingly rare); clearly there is scope to improve operational efficiencies in such a case to reduce energy usage and the associated GHG emissions. Practical steps to increase operational efficiencies include the

installation of dissolved oxygen (DO) monitoring and control in aerated tanks to reduce energy used for aeration; change in or reduction of pumping operations; improved management of storage tanks in sewer system to level the WWTP loading; installation of adjustable-speed drives on pumps and blowers for variable flow operations; and use of on-line sensors to monitor sewage components such as BOD and suspended solids and mixing of streams as necessary to maintain constant loading. Additionally, discharge quality could be altered depending on the capacity of the receiving waters to self-clean without adverse environmental impacts (subject to meeting legislative standards).

Currently, schemes for increasing energy efficiencies are being proposed and implemented with little consideration of the effect that they will have on overall system performance or their interaction with each other (Ainger et al. 2009). However, carrying out holistic water quantity and quality analysis with consideration for energy consumption as a result of wastewater conveyance and treatment (instead of designing and operating wastewater infrastructure components independently) could result in increased operational efficiencies.

Renewable Energy Generation

Energy can be generated from waste. Biogas emitted during anaerobic solids digestion and containing CH_4 , for example, has a significant potential energy of 24MJ/m^3 (WEF and ASCE 1998).

A major benefit of energy recovery from biogas is that the CH_4 is converted to CO_2 when combusted, therefore reducing the GWP of the emissions. It also results in a reduction in GHG emissions associated with offsite energy generation, as less imported electricity is required. In large plants, biogas from anaerobic digesters can be used to provide fuel for boilers or internal combustion engines, which might provide power for generating electricity, pumping wastewater or operating blowers. Additional uses might include vehicle fuel and heating sludge and/or buildings.

Renewable energy generation from biogas is already common practice (although, where not cost effective, the biogas is sometimes flared); however, operational procedures could potentially be modified to maximise CH_4 production in the anaerobic digester, thereby increasing production of 'green' energy and reducing or eliminating the need for imported electricity.

Change of Operational Procedures

Where CH₄ is not captured for renewable energy generation, emissions can be reduced by maintaining aerobic conditions (greater than 0.2 – 0.6 mg/L of oxygen (Loehr 1984)). To achieve this, the U.S. Environmental Protection Agency (USEPA) (1993) recommend using aerobic primary and secondary treatment (instead of anaerobic). They also highlight the importance of controlling the organic loading and providing additional oxygen by mechanical aeration in order to maintain sufficient levels of oxygen in the aerobic reactor.

However, a key disadvantage of operating under aerobic conditions is that, whilst significantly reducing carbon emissions, the operating cost is greater due to the additional energy required for aeration. Additionally, aerobic processes result in high sludge production, which must be properly managed to avoid CH₄ emissions. It has therefore been suggested that anaerobic digestion with CH₄ recovery could be adopted to minimise both GWP and cost (El-Fadel and Massoud 2001). The recovered CH₄ can then be used as an energy source (as discussed previously). Alternatively, if the CH₄ generation is insufficient to warrant construction of an energy recovery system, the CH₄ may be ignited (flared) so that the primary emission is CO₂, which has a lower GWP.

During sludge treatment and disposal, the USEPA (1993) suggest that CH₄ emissions could be reduced by a number of procedures, including chemical stabilisation, aerobic composting, land application, incineration, landfilling with CH₄ recovery or perhaps other experimental uses for sludge.

1.3 Aims and Objectives

The aim of this research is to ***develop strategies for the reduction of greenhouse gas emissions from wastewater treatment processes***, utilising multi-objective optimisation techniques to reduce emissions resulting from the operation of wastewater treatment plants whilst taking into account alternative drivers and conflicting objectives.

As the name suggests, the CRC only covers emissions associated with energy use – GHGs such as those formed by biological processes in wastewater treatment, for example, are not accounted for. However, this research is not restricted to just energy related emissions, since from an environmental

perspective it is better to minimise total GHG emissions. If a net reduction is achieved, whether or not this is reflected in the reported figures is irrelevant in terms of the effects on global warming. A low energy solution that appears desirable based on the CRC requirements may result in an increase in net emissions, which would clearly be undesirable. As such, this study aims to develop strategies for the reduction of total GHG emissions, although the effects of this on emissions which companies are required to report is investigated also.

The strategy development process is to focus on achieving optimal control of existing systems, without extensive redesign. Strategies must be suitable for use with time varying inputs, and strategy design processes must be applicable to different systems. Further challenges are posed by future uncertainties such as urbanisation and the impacts of climate change, and there is a need to assess the robustness and resilience of any control strategies devised.

In order to achieve this aim, a number of objectives have been identified:

1. Develop or adapt a WWTP model to enable assessment of direct and indirect operational GHG emissions under dynamic loading, in addition to WWTP performance with respect to treatment standards.
2. Develop and optimise control strategies to reduce GHG emissions whilst maintaining required treatment standards, and investigate trade-offs between emissions, cost and effluent quality.
3. Investigate the effects of developing control strategies to reduce total GHG emissions on emissions which companies are compelled to report.
4. Investigate the impact of optimisation on the reliability, resilience and robustness of control strategies and explore measures to improve these.
5. Identify control strategy features that contribute to a reduction in GHG emissions and use to generate guidelines for WWTP operation and control strategy development to reduce emissions.

1.4 Scope

The research is split into seven components: a literature review; model development; identification of key sources of uncertainty in the modelling of GHG emissions; identification of sensitive sources and key control handles for emission reduction; control strategy development; investigation into the reliability, robustness and resilience of optimised control strategies; and production of control strategy development guidelines. Interaction between these components and their contribution to achievement of the study objectives is shown in Figure 1.1. Tasks undertaken for completion of each objective are summarised in Sections 1.4.1-1.4.5.

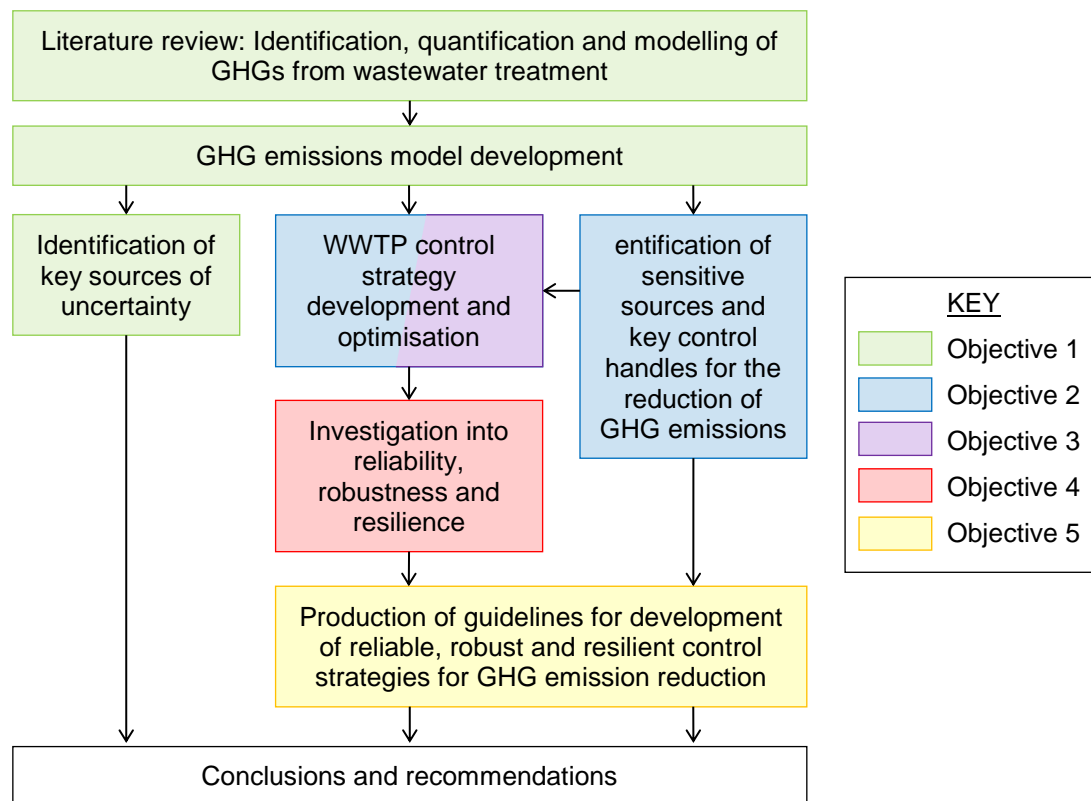


Figure 1.1: Interactions between thesis components and connection with objectives

1.4.1 Model Development

- a) Identify legislation relating to GHG emissions from WWTPs and development of control strategies (e.g. emissions reporting and reduction requirements, effluent quality standards and performance monitoring).

- b) Identify sources of GHG emissions in wastewater treatment and investigate scope and limitations of existing methods of calculation.
- c) Integrate emission modelling methodologies in a single WWTP model, ensuring the model has capacity to support system parameters and control handles which may be required for control strategy development.
- d) Carry out sensitivity analysis to detect model parameters whose accuracy has the greatest/least effects on model outputs and inform future uncertainty analyses.

1.4.2 Control Strategy Development

- a) Research WWTP control strategy development and previously proposed control strategies and use of control handles and sensors.
- b) Assess the GHG emissions resulting from previously proposed control strategies, and the associated effluent quality and operational costs.
- c) Identify the most significant sources of GHG emissions and use sensitivity analysis to identify control handles to which GHG emissions, effluent quality and operational costs are most sensitive.
- d) Research tools for multi-objective optimisation and select suitable methods for control strategy development and optimisation.
- e) Select simple base control strategy/strategies and carry out optimisation to minimise GHG emissions, operational costs and effluent pollutant load.
- f) Investigate opportunity for further improvements using either more sophisticated or simpler control strategies as appropriate.
- g) Compare performance of optimised / proposed control strategies with that of a base case scenario.

1.4.3 Total and Reported Emissions

- a) Calculate magnitude of emissions companies are compelled to report resulting from optimised control strategies
- b) Investigate relationships and/or trade-offs between emissions which companies are compelled to report and total GHG emissions.

1.4.4 Reliability, Robustness and Resilience

- a) Research definitions and measures of reliability, robustness and resilience, and select or develop methodology for assessment of each.
- b) Assess the reliability, robustness and resilience of optimised control strategies developed under Objective 2.
- c) Investigate relationships between control strategy features (either in terms of performance or in control variables) and reliability, robustness and resilience, and identify methods of control strategy development or selection to improve these performance indicators.

1.4.5 Design Guidelines

- a) Identify any common features in control strategies that result in a reduction in GHG emissions.
- b) Identify and analyse any relationships between decision variable values and performance indicators, including GHG emissions.
- c) Investigate features contributing to a reliable, robust and resilient (or an unreliable, non-robust and non-resilient) design.
- d) Develop generic design guidelines for WWTP operation and the development of control strategies to reduce GHG emissions at an acceptable cost whilst maintaining legislative compliance.

1.5 Thesis Structure

The thesis contains nine chapters, which correspond with the stages shown in Figure 1.1 and achievement of the objectives. These are as follows:

Chapter 1: Introduction and scope

Background information is presented and the aims and objectives of the research detailed. The originality and contribution to knowledge provided by the thesis are also highlighted.

Chapter 2: Identification, quantification and modelling of greenhouse gas emissions from wastewater treatment

The literature review identifies GHG emission sources and provides an in-depth analysis of methods and models for estimating GHG emissions from WWTPs, focussing primarily on emissions arising due to biological processes and energy consumption. The methods and models identified are analysed with respect to their suitability for dynamic modelling of WWTPs for control strategy optimisation.

This chapter contains research presented at the IWA UK Young Water Professionals' Conference 2012 (Sweetapple 2012):

Sweetapple, C. (2012) Estimation of greenhouse gas emissions for development of adaptive wastewater treatment plant carbon management strategies: A literature review. In 13th IWA UK Young Water Professionals Conference, 18-20 April 2012, Exeter, UK

Chapter 3: Greenhouse gas emissions model development

An emissions model developed by implementation of existing methodologies in the Benchmark Simulation Model No. 2 (BSM2) (Jeppsson et al. 2007) is presented. This model enables assessment of dynamic GHG emissions under different control options and provides the basis for work in the following chapters.

This chapter is based on the model description given in the following publication, but with significant additional detail (Sweetapple et al. 2013):

Sweetapple, C., Fu, G. and Butler, D. (2013) Identifying key sources of uncertainty in the modelling of greenhouse gas emissions from wastewater treatment. *Water Research* 47(13), 4652-4665.

Chapter 4: Identifying key sources of uncertainty in the modelling of greenhouse gas emissions from wastewater treatment

Sources of uncertainty are investigated through the use of local and global sensitivity analysis (GSA) tools, revealing critical parameters and parameter interactions. One-factor-at-a-time (OAT) sensitivity analysis is used to screen model parameters and identify those with significant

individual effects on three performance indicators: total GHG emissions, effluent quality and operational cost. Sobol's method enables identification of parameters with significant higher order effects and of particular parameter pairs to which model outputs are sensitive.

This chapter is based upon the following publication (Sweetapple et al. 2013):

Sweetapple, C., Fu, G. and Butler, D. (2013) Identifying key sources of uncertainty in the modelling of greenhouse gas emissions from wastewater treatment. *Water Research* 47(13), 4652-4665.

Chapter 5: Identifying sensitive sources and key control handles for the reduction of greenhouse gas emissions

The effects of adjusting control handle values on GHG emissions are investigated using local and global sensitivity analysis, and critical control handles and sensitive emission sources for control are identified. Sources with the greatest variance in emissions, and therefore the greatest need to monitor, are also revealed.

This chapter is based upon the following publication (Sweetapple et al. 2014a):

Sweetapple, C., Fu, G. and Butler, D. (2014a) Identifying sensitive sources and key control handles for the reduction of greenhouse gas emissions from wastewater treatment. *Water Research* 62, 249-259.

Chapter 6: Wastewater treatment plant control strategy development and optimisation

The potential of control strategy optimisation for the reduction of operational GHG emissions is investigated, using a multi-objective evolutionary algorithm to derive sets of Pareto optimal operational and control parameter values. Objectives considered include minimisation of GHG emissions, operational costs and effluent pollutant concentrations, subject to legislative compliance. Different problem formulations are explored, to identify the most effective approach to emissions reduction,

and the sets of optimal solutions enable identification of trade-offs between conflicting objectives.

Implementation of alternative control strategies is also investigated, with key control handles identified in Chapter 5 sampled to provide sets of values for testing in two pre-defined control strategies.

This chapter is based upon the following publications (Sweetapple et al. 2014b, Sweetapple et al. 2014c):

Sweetapple, C., Fu, G. and Butler, D. (2014b) Multi-objective optimisation of wastewater treatment plant control to reduce greenhouse gas emissions. *Water Research* 55, 52-62.

Sweetapple, C., Fu, G.T. and Butler, D. (2014c) Cost-efficient control of wastewater treatment plants to reduce greenhouse gas emissions. In *IWA World Water Congress & Exhibition*, 21-26 September 2014, Lisbon, Portugal.

Chapter 7: Investigating the impact of control strategy optimisation to reduce greenhouse gas emissions on reliability, robustness and resilience

Definitions and means of quantifying reliability, resilience and robustness are explored and then, using chosen measures, a sample of optimised control strategy solutions derived in Chapter 6 are assessed with respect to their ability to maintain a compliant effluent and acceptable GHG emissions under predefined disturbances or ‘threats’.

Relationships between control strategy design, performance (in terms of GHG emissions, operational costs and effluent quality), reliability, robustness and resilience are explored, and the impacts of control strategy optimisation investigated.

Chapter 8: Guidelines for the development of control strategies to reduce greenhouse gas emissions

This chapter draws upon the findings in Chapters 4-7 to produce guidelines for the development of control strategies to reduce GHG emissions from wastewater treatment in a cost-effective manner whilst maintaining a compliant effluent. Given that the WWTP model used in the

research is of a hypothetical plant and that there are (necessarily) omissions in the sources of GHG emissions included, no single specific 'best' control strategy is proposed – rather, general recommendations are made based on observed trends.

Chapter 9: Conclusions and recommendations

This draws upon the previous chapters to present the key research findings and discuss recommendations for future work.

1.6 Originality and Contribution to Knowledge

This thesis has:

- Contributed to an in-depth understanding of wastewater treatment modelling by revealing critical parameters and parameter interactions contributing to uncertainty in the modelling of GHG emissions. Use of a variance-based GSA tool to investigate parameter interactions has enabled identification of important parameters not identified in OAT sensitivity analysis. These interaction effects have not been considered in previous studies and thus provide a better understanding wastewater treatment plant model characterisation. (*Chapter 4*)
- Identified control handles to which GHG emissions, effluent quality and operational costs are sensitive. The direction of change in each performance indicator resulting from variation of control handles individually was determined using OAT sensitivity analysis, and corresponding trade-offs identified. The contribution of each control handle to variance in model outputs, taking into account the effects of interactions, was explored using a variance-based sensitivity analysis method and significant second order interactions discovered. This knowledge will assist future control strategy development and aid an efficient design and optimisation process, as it provides a better understanding of the effects of control handles on key performance indicators and identifies those for which dynamic control has the greatest potential benefits. (*Chapter 5*)
- Identified sources of GHG emissions with the greatest scope for improvement (or potential for adverse effects) by adjustment of WWTP

control alone, by analysis of variance of GHG emissions from each source when subject to control handle adjustments. (*Chapter 5*)

- Demonstrated the potential of control strategy optimisation for the reduction of GHG emissions from wastewater treatment at an acceptable cost whilst maintaining a compliant effluent. It is shown that multi-objective optimisation can facilitate a significant reduction in GHG emissions without the need for plant redesign or modification of the control strategy layout, but there are trade-offs to consider and these are explored. (*Chapter 6*)
- Shown that significant reduction in GHG emissions and operational costs can be realised by implementation of an appropriate control strategy and improved selection of operational parameter values. (*Chapter 6*)
- Highlighted the importance of considering GHG emissions in control strategy selection, given that different control strategies are observed to produce effluent of a similar quality but with significantly different emissions. (*Chapter 6*)
- Investigated the impact of optimisation on the reliability, robustness and resilience of control strategies with regard to effluent quality and GHG emissions when subject to changes in influent conditions and sensor failures. This enables different solutions providing acceptable reliability, robustness and resilience to be identified and control features contributing to a preferable solution identified. (*Chapter 7*)
- Developed guidelines for the development of reliable, robust and resilient control strategies to reduce GHG emissions resulting from the operation of wastewater treatment processes. (*Chapter 8*)

2 LITERATURE REVIEW: IDENTIFICATION, QUANTIFICATION AND MODELLING OF GREENHOUSE GAS EMISSIONS FROM WASTEWATER TREATMENT

In order to develop a model that can be used to optimise control strategies for the reduction of GHG emissions, it is necessary to first identify appropriate emission estimation methods. Many existing approaches are based on empirical formulae, using steady state calculations; however, whilst these can provide a useful indication of the likely emissions, they are unsuitable for use in optimisation as they do not allow for the effect of changing operating conditions and influent loads to be modelled. Models used must also allow the contribution of individual processes to direct and indirect GHG emissions to be determined.

In this chapter, therefore, a review of GHG emissions resulting from wastewater treatment processes, methods by which these can be estimated and existing emission models is presented.

2.1 Greenhouse Gas Emission Sources

Several authors (e.g. Stokes and Horvath 2009, Rothausen and Conway 2011) advocate the use of life cycle assessment (LCA) to inform decision making with respect to carbon management in the water sector. The life cycle can be viewed both in terms of the plant (construction, operation, maintenance and disposal) and the water (abstraction and conveyance, treatment and distribution, end use and wastewater treatment). However, this can pose challenges, as the approach taken for reducing emissions can differ in each stage of the life cycle and not all aspects can be controlled by water companies to the same extent. For example, demand management can be used to help lower emissions associated with end use, but the consumers' water consumption habits are largely beyond the control of the water industry. Given that this research focusses on improving the control of existing systems rather than the development of new, improved WWTPs, a complete LCA is of little benefit and assessment of GHG emissions is based on just those associated with operation of the WWTP.

Emissions can be categorised as either 'direct' or 'indirect', depending on their source. Direct emissions are those which are emitted at the point of use and from a source that is either owned or controlled by the reporting entity.

Wastewater treatment processes can result in the production of CO₂, CH₄ and N₂O, and further direct emissions may result from the combustion of fuels or fugitive emissions such as CH₄ leaks from pipes. Emissions from a source not owned or controlled by the reporting entity but which occur as a result of their activities are classified as indirect emissions. In the context of a WWTP, these include emissions associated with the generation of electricity for onsite use, processing of chemicals and waste disposal.

Emissions may also be categorised depending on whether they are of biogenic or non-biogenic origin. Current accounting guidelines for GHG emissions assume all organic carbon to be of biogenic origin (IPCC 2006b) and do not, therefore, require any CO₂ emissions to be recorded. However, it has been found that up to 14% of the total organic carbon in raw wastewater is of fossil origin (i.e. not biogenic) and over 6% of the influent total organic carbon may be transformed to fossil CO₂ (Law et al. 2013). It has consequently been suggested that assumption that all CO₂ emissions are of biogenic origin may result in underestimation of emissions (Law et al. 2013). Given that the aim of this research is to reduce total GHG emissions, however, whether this is achieved through reduction of emissions of biogenic or non-biogenic origin is irrelevant; no distinction is made and no emissions are overlooked on the basis of their origin.

2.1.1 Direct Emissions

Within the water industry, particular attention must be paid to emissions associated with the collection, treatment and disposal of wastewater and disposal of sludges, in addition to those resulting from energy consumption. It is thought that direct GHG emissions from wastewater treatment could be of a similar magnitude to those from the use of energy; however there is currently a high level of uncertainty for data such as CH₄ emissions from reservoirs (Hall et al. 2011).

Secondary treatment, for example, typically employs biological processes. These utilise micro-organisms to remove dissolved and suspended organic matter in wastewater and may be carried out either aerobically or anaerobically, resulting in emissions of CO₂ and/or CH₄.

An overview of the processes resulting in direct emission of GHGs in the wastewater system is given in the following sections. Details of recent studies into factors affecting the rate of emission and methods of estimating emissions are given where appropriate. However, all emission estimation methods are associated with a degree of uncertainty, depending on the availability and accuracy of information on wastewater generation rates, the degradable organic fraction and spatial and temporal variations.

Methane Production and Emission

In the urban water system, significant volumes of CH₄ can be formed in the sewerage system under anaerobic conditions before entry to the WWTP (Guisasola et al. 2009) and it is thought that this may contribute significantly to total GHG emissions from wastewater systems. Although the impact of CH₄ formation in sewers is not commonly considered when estimating GHG emissions from WWTPs, Guisasola et al. (2008) suggested that dissolved CH₄ may come out of solution at a pressure drop in the system and it is highly likely to be stripped from the wastewater when entering a WWTP. This theory is supported by measurements made at a full-scale plant in China by Wang et al. (2011), where CH₄ emissions were observed at the influent pump station.

Within the WWTP boundary, CH₄ production is most significant during anaerobic digestion. When treatment is carried out under anaerobic conditions (most commonly for waste sludge and high strength organic wastes), the biogas produced contains approximately 56 - 70 % CH₄ and 25 - 30 % CO₂ by volume (Metcalf and Eddy 1994) and has a substantial CO₂e.

Biogas formed during anaerobic digestion is rarely deliberately released into the atmosphere, but it is necessary to estimate production in order to calculate energy recovery and CO₂ emissions from CH₄ combustion. There may also be biogas leaks – typically assumed to be in the order of 5 % (Georges et al. 2009, Shahabadi et al. 2009) – which contribute to overall CH₄ emissions.

Theoretical and experimental approaches have been taken to create methodologies for the estimation of CH₄ production during anaerobic biodegradation of the organic fraction in wastewater and a range of emission factors have been proposed.

UKWIR (2008, quoted in Georges et al. 2009) proposed an emission factor of 18 kg CH₄/tonne sludge (raw, dry solids) treated. Alternatively emissions can be estimated on a per capita basis: the biogas emission factor and typical biogas composition given by Metcalf and Eddy (1994) yields a CH₄ emission factor of 10.59 - 13.24 g CH₄/person/year. However there is a high degree of uncertainty when using this method. Per capita emission factors measured at some WWTPs are within this range (e.g. Wang et al. 2011), but others differ considerably; a study by Czepiel et al. (1993), for example, recorded an emission factor of 39 g CH₄/person/year at a WWTP in Durham (UK), which is significantly higher.

The results of a recent investigation into CH₄ emissions from a large WWTP (Wang et al. 2011) were presented in terms of CH₄ emitted per unit area. Emissions were observed in every processing unit, with emission factors ranging from 0.11 to 978 g CH₄/m²/day. This can be misleading however, as some of the processing units with the greatest emission factors had the smallest surface areas, and therefore did not provide the greatest contribution to emissions. Taking into account surface areas, the anaerobic tanks and oxic tanks had the greatest annual CH₄ emissions. Emissions factors were also calculated with respect to the volume of wastewater treated, giving 0.129 - 0.203 g CH₄/m³. In the study, it was assumed that these emission factors could be applied to all municipal WWTPs in China; however, as Chinese WWTPs are much larger than many used in other research investigations (Wang et al. 2011), it is inappropriate to apply the emission factors when assessing WWTPs in other countries.

Whilst emission factors given in terms of population or volume of wastewater treated can provide a useful estimation of CH₄ emissions, a more detailed methodology would be required for development and optimisation of carbon management strategies, as demand management is beyond the scope of this research project. Per capita emission factors are unsuitable for dynamic modelling due to their empirical nature and questionable reliability; they do not reflect the effect of changing wastewater composition on CH₄ emissions, instead suggesting that reductions can only be achieved by reducing demand. The study by Wang et al. (2011) provided a detailed analysis of the contribution of each processing unit to overall CH₄ emissions, but again the calculated per

unit area emission factors could not be meaningfully applied to other WWTPs or used for modelling; optimisation on this basis would suggest that the surface area simply needs to be reduced. Instead a rational method of calculating emissions on a site-specific basis is required.

The main factor influencing the extent of CH₄ production in anaerobic treatment is the mass of degradable organic material in the wastewater, expressed in terms of biochemical oxygen demand (BOD) or chemical oxygen demand (COD); under the same environmental conditions, CH₄ yield will increase as BOD or COD increases (El-Fadel and Massoud 2001).

The anaerobic oxidation of waste involves three stages: hydrolysis, fermentation and methanogenesis (Metcalf and Eddy 1994). During hydrolysis, particulate material is converted to simple monomers that can be fermented by bacteria. In the fermentation step, organic substrates are further degraded, resulting in the production of hydrogen, CO₂ and acetate. These products are used by methanogenic organisms in the final step, methanogenesis, to produce CH₄.

Metcalf and Eddy (1994) suggested that CH₄ emissions could be estimated using Eq. 2.1, based on BOD reduction and an appropriate emission factor:

$$V_{CH_4} = (EF)[(S_0 - S)(Q)(10^3 g/kg)^{-1} - 1.42P_x] \quad \text{Eq. 2.1}$$

where:

- V_{CH_4} = volume of CH₄ produced [m³]
- EF = emission factor for the volume of CH₄ produced [m³] from the conversion of 1kg of BOD
- Q = flow rate [m³/d]
- S_0 = BOD in influent [mg/L]
- S = BOD in effluent [mg/L]
- P_x = net mass of cell tissue produced per day [kg/d], estimated using Eq. 2.2

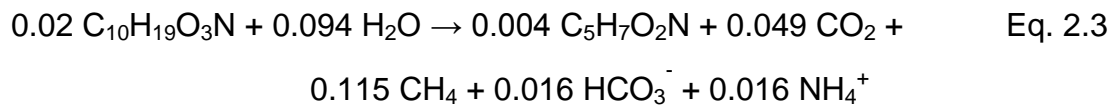
$$P_x = \frac{YQ(S_0 - S) \times (10^3 g/kg)^{-1}}{1 + k_d(SRT)} \quad \text{Eq. 2.2}$$

where:

- Y = yield coefficient [g VSS/g BOD]

k_d = endogenous decay coefficient [d^{-1}]
 SRT = solids retention time [d]

Emission factors proposed for use in Eq. 2.1, however, vary greatly. Shahabadi et al. (2010) stated that carbonaceous substrate utilisation under anaerobic conditions results in the formation of CO_2 and CH_4 as shown in Eq. 2.3, and using stoichiometry to calculate the COD equivalent of CH_4 implies that production under anaerobic conditions should be 0.35 L CH_4 /g COD at 0°C and 1 atm, increasing to 0.40 L CH_4 /g COD at 35°C (Metcalf and Eddy 1994) (equivalent to 0.25 g CH_4 /g COD in both cases).



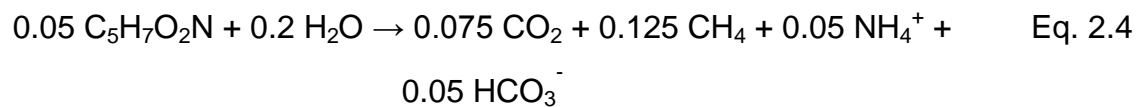
However, emission factors as low as 0.1 g CH_4 /g COD have been observed in field tests (Toprak 1995). This suggests that any emissions estimated using this method would be of questionable accuracy. Variations in CH_4 production could be attributed to a number of factors for which no allowance is made in Eq. 2.3, including temperature, pH and presence of toxicants. To address this, the IPCC (2006b) provided a methodology for estimating CH_4 emissions from a range of treatment processes based on maximum CH_4 producing capacity as determined from stoichiometry and a CH_4 correction factor.

This includes aerobic processes with unintentionally anaerobic conditions in addition to anaerobic processes and yields default emission factors ranging from 0.0 - 0.2 g CH_4 /g COD consumed, as summarised in Table 2.1. However, whilst these emission factors may provide a more accurate representation of CH_4 emissions, they are still limited in their application to dynamic modelling as they do not provide a quantifiable relationship between the correction factor and operational parameters affecting emissions. For example different emission factors are given for well managed and poorly managed aerobic treatment but the relationship between management standard and operational parameters such as DO concentration is not defined. Additionally, the transition from good to poor management is unclear, as there is a gap in the emission factors.

Table 2.1: Emission factors based on default maximum CH₄ producing capacity and CH₄ correction factors given by the IPCC (2006b)

Type of treatment		Emission factor range					
		g CH ₄ /g BOD			g CH ₄ /g COD		
		Lower	Default value	Upper	Lower	Default value	Upper
Aerobic	Well managed, centralised aerobic treatment plant	0.00	0.00	0.06	0.00	0.00	0.03
	Poorly managed and overloaded, centralised aerobic treatment plant	0.12	0.18	0.24	0.05	0.08	0.10
Anaerobic	Anaerobic digester for sludge	0.48	0.48	0.60	0.20	0.20	0.25
	Anaerobic reactor	0.48	0.48	0.60	0.20	0.20	0.25
	Anaerobic shallow lagoon	0.00	0.12	0.18	0.00	0.05	0.08
	Anaerobic deep lagoon	0.48	0.48	0.60	0.20	0.20	0.25

Shahabadi et al. (2010) noted that CH₄ may also be produced during biomass decay under anaerobic conditions, in accordance with Eq. 2.4:



This yields a theoretical emission factor 0.35 g CH₄/g VSS decayed. Again, use of this emission factor does not take into account the effect that other process parameters may have on biomass decay and simply provides the maximum theoretical yield. Metcalf and Eddy (1994) suggested that emissions vary within the range 0.75 - 1.12 L CH₄/g VSS (equivalent to 0.53 - 0.80 g CH₄/g VSS assuming 0°C and 1 atm). These values are significantly higher than the theoretical maximum and are therefore of questionable accuracy; it is possible that they are intended for use in estimating total CH₄ emissions from biological processes, i.e. biomass decay and BOD oxidation, using only volatile suspended solids (VSS) data.

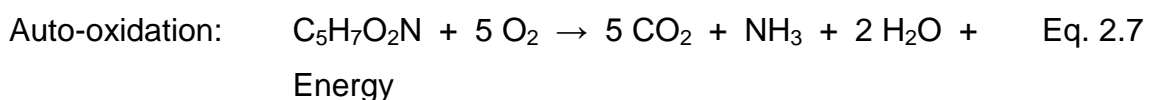
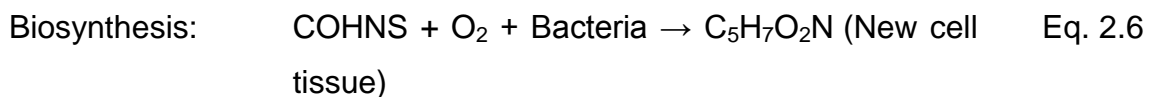
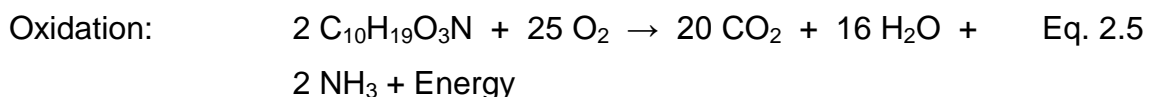
Shahabadi et al. (2010) also highlighted that a fraction of the CH₄ produced in the anaerobic reactor and digester will remain dissolved in the effluent and therefore the CH₄ content of biogas will be less than the total CH₄ production.

Within the WWTP boundary, anaerobic conditions occur primarily in anaerobic reactors and anaerobic digesters. However, it has been noted that other processes, such as holding tanks, may be unintentionally anaerobic and sludge may be stored under anaerobic conditions, resulting in further CH₄ emissions to the atmosphere (El-Fadel and Massoud 2001, Monteith et al. 2005). This theory is supported by experimental evidence, as CH₄ emissions from were observed at every processing unit in a recent full-scale investigation (Wang et al. 2011).

Carbon Dioxide Production and Emission

Both aerobic and anaerobic wastewater treatment processes result in CO₂ emissions, although aerobic treatment inhibits CH₄ production. If emissions are to be released directly into the atmosphere then this scenario is preferable as CO₂ has a significantly lower GWP than CH₄.

In the presence of oxygen, two distinct processes are used by micro-organisms to break down the organic matter: biological oxidation and biosynthesis. If the availability of oxygen becomes limited then auto-oxidation (endogenous respiration) of biomass will occur. These three processes occur simultaneously and can be expressed as follows (Monteith et al. 2005, Gray 2010):



Monteith et al. (2005) suggested that steady state CO₂ emissions from aerobic wastewater treatment could be estimated based on calculation of the total theoretical mass of BOD converted to biomass under aeration and the oxygen requirement, using Eq. 2.8 and Eq. 2.9 respectively. Eq. 2.8 is derived from a suspended solids mass balance (Eq. 2.10), assuming that the primary clarifier

sludge flow rate is negligible in comparison with the influent wastewater flow rate.

$$YVr_s = Q_wX_r + (Q_i - Q_w)X_c + VK_dX - f_{nd}Q_iX_{pc} \quad \text{Eq. 2.8}$$

$$r_{O_2} = Vr_s \left(\frac{1}{f} - 1.42Y \right) \quad \text{Eq. 2.9}$$

$$V \left(\frac{dX}{dt} \right) = f_{nd}(Q_i - Q_{pc})X_{pc} + YVr_s - Q_wX_r - (Q_i - Q_{pc} - Q_w)X_e - VK_dX \quad \text{Eq. 2.10}$$

where:

- f = ratio of BOD₅ to ultimate BOD (BOD_u), typically 0.68 (Metcalf and Eddy 1991)
- f_{nd} = fraction of VSS entering aeration basin from primary clarifier that are not degraded (used as a fitting term)
- k_d = biomass endogenous decay coefficient [d⁻¹]
- r_{O_2} = oxygen removal rate [g O₂/d]
- r_s = aeration BOD₅ removal rate [g BOD₅/m/d]
- Q_i = influent wastewater flow rate [m³/d]
- Q_w = waste biomass flow rate [m³/d]
- Q_{pc} = primary clarifier sludge flow rate [m³/d]
- V = aerobic reactor volume [m³]
- X = biomass concentration in aerobic reactor [g VSS/m³]
- X_e = effluent VSS [g VSS/m³]
- X_{pc} = VSS in primary clarifier effluent [g VSS/m³]
- X_r = return biomass concentration [g VSS/m³]
- Y = cell yield coefficient [g VSS/g BOD₅]

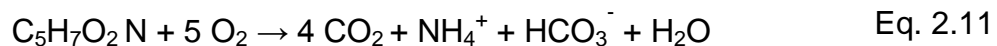
A rational procedure can then be used to apportion the mass of BOD converted by each of the three aerobic processes (oxidation, biosynthesis and auto-oxidation) and stoichiometry used to derive emission factors:

- Eq. 2.5 predicts that, during oxidation, 0.8 moles of CO₂ are released for every mole of oxygen consumed; using molecular weights therefore yields a conversion factor of 1.1 kg CO₂/kg O₂. The oxygen consumed is calculated using Eq. 2.9.

- During biosynthesis (Eq. 2.6), no CO₂ is produced.
- During auto-oxidation, 1 mole of biomass releases 5 moles of CO₂ (as shown in Eq. 2.7); molecular weights can therefore be used to derive a conversion factor of 1.947 kg CO₂/kg VSS for estimation of carbon emissions resulting from auto-oxidation of biomass (Monteith et al. 2005). Of the total BOD converted to biomass under aeration (Eq. 2.8), the mass converted to CO₂ by auto-oxidation is given by VK_dX .

A limitation of this method for estimation of GHG emissions is that it assumes aerobic conditions are maintained and only CO₂ is produced, despite identifying that CH₄ may be produced under certain conditions (for example when deep sludge blankets form as a result of inadequate underflow removal). The justification given is that, as the CH₄ production is unintentional and a result of poor design or operation, it cannot be predicted with any certainty.

Furthermore, there are discrepancies in the stoichiometric relationships used to express the process of auto-oxidation in different estimation methodologies. Shahabadi et al. (2010), for example, assumes auto-oxidation can be expressed by Eq. 2.11. This leads to a conversion factor of 1.556 g CO₂/g VSS, which is a 20% reduction from that calculated by Monteith et al. (2005).



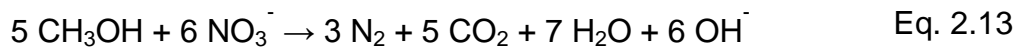
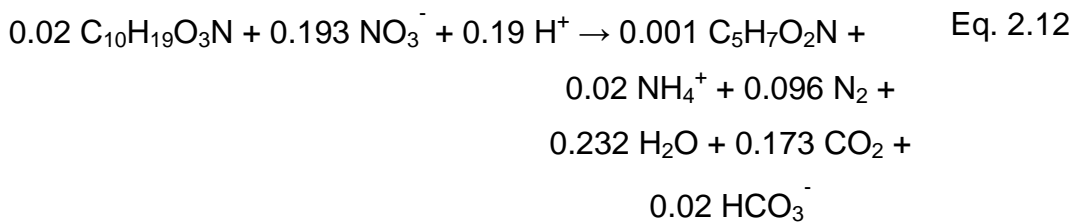
Aerobic treatment may be used for sludge as well as wastewater, resulting in further CO₂ emissions. Many methods published for estimation of GHG emission from WWTPs do not consider emissions from aerobic digestion and it is assumed that only anaerobic digestion is used (Cakir and Stenstrom 2005, Shahabadi et al. 2009, Flores-Alsina et al. 2011, Gori et al. 2011). However, Monteith et al. (2005) assume that the BOD conversion processes are the same as in wastewater treatment (Eq. 2.5 - Eq. 2.7) and CO₂ emissions can be calculated in a similar manner, based on stoichiometry and using the mass of BOD converted and the oxygen requirement.

In order to estimate CO₂ emissions from anaerobic treatment processes, previous methodologies have assumed that anaerobic digester biogas contains fixed proportions of CO₂ and CH₄ (Monteith et al. 2005); however, this approach cannot reasonably be applied in dynamical modelling. Firstly it requires an

accurate calculation of the volume of biogas produced – Monteith et al. (2005) use an emission factor (m^3 gas produced / g VSS destroyed), but this does not take into account the effect of variables other than VSS removal on gas production. Additionally, this approach to estimating CO_2 emissions from anaerobic treatment assumes that the composition of biogas is constant, but Metcalf and Eddy (1994) noted that CO_2 content typically ranges from 25 - 30%.

Shahabadi et al. (2010) instead calculated CO_2 production from BOD utilisation and biomass decay in the anaerobic reactor using stoichiometry: Manipulation of Eq. 2.3 and Eq. 2.4 yields emission factors of $0.27 \text{ g CO}_2/\text{g BOD}$ and $0.58 \text{ g CO}_2/\text{g VSS}$ respectively. Use of this method provides the theoretical maximum CO_2 production.

Nutrient removal may generate additional GHG emissions (Shahabadi et al. 2010). Denitrification in an aerobic environment, for example, leads to the formation of CO_2 . Shahabadi et al. (2010) state that the denitrification process can be expressed by Eq. 2.12 if no external carbon source is used or by Eq. 2.13 if methanol is added (the impact of pH is not discussed). Examination of molar masses, however, shows that Eq. 2.12 is unbalanced ($16.18 \text{ g} \rightarrow 15.85 \text{ g}$) and therefore cannot be an entirely accurate representation of the denitrification process.



As with aerobic and anaerobic processes, CO_2 production during denitrification can be estimated using stoichiometry. If the use of Eq. 2.12 and Eq. 2.13 to represent denitrification is assumed to be valid, then emission factors of $2.62 \text{ g CO}_2/\text{g N-nitrate}$ and $2.81 \text{ g CO}_2/\text{g N-nitrate}$ for denitrification with and without an external carbon source respectively can be derived (Shahabadi et al. 2010). Use of this method, however, assumes that complete denitrification is achieved and no N_2O is emitted as an intermediate product.

During biological nutrient removal, CO₂ is also consumed in the process of nitrification (Metcalf and Eddy 1994), therefore reducing net CO₂ emissions. Flores-Alsina et al. (2011) used a factor of 0.31 kg CO₂/kg N to calculate the CO₂ credit from nitrification.

Direct CO₂ emissions also occur during the combustion of biogas produced during anaerobic digestion. Biogas has a high potential energy and is commonly combusted for heating or electricity generation. This results in the conversion of CH₄ and oxygen to CO₂ and water, which is preferable due to the lower GWP of the emissions (Monteith et al. 2005). Whilst it is established practice to exclude CO₂ from renewable sources when reporting emissions (El-Fadel and Massoud 2001), production can be estimated directly in terms of the mass of sludge processed using an emission factor of 25.4 kg CO₂/tonne of sludge treated (UKWIR 2005, quoted in Georges et al. 2009). Alternatively, the CO₂ production can be calculated using the chemical reaction for oxidation of CH₄, Eq. 2.14.



From this it can be derived that 2.75 kg CO₂ is released for every 1 kg CH₄ oxidised (Monteith et al. 2005, Shahabadi et al. 2010).

However, there is considerable discrepancy between the results obtained from different methods: using emission factors of 18 kg CH₄/tonne of sludge treated (UKWIR 2008, quoted in Georges et al. 2009) and 2.75 kg CO₂/kg of CH₄ oxidised suggests that combustion of biogas would result in CO₂ emissions of 49.5 kg CO₂/tonne of sludge treated – nearly double the emission factor given by UKWIR (2005, quoted in Georges et al. 2009). Errors may also be introduced when using Eq. 2.14 as it requires either knowledge or an assumption of the proportion of CH₄ in the biogas which is fully oxidised.

Nitrous Oxide Production and Emission

The degradation of nitrogen components in wastewater, such as urea, nitrate and protein, can result in the formation of N₂O (IPCC 2006b).

N₂O emissions result from heterotrophic denitrification and autotrophic nitrification (Wunderlin et al. 2012). Denitrification is the reduction of nitrate to nitrogen – a four step process in which N₂O is an intermediate product.

Nitrification is the process by which ammonia is converted into nitrite by ammonium-oxidising bacteria (AOB) and ammonium-oxidising archaea and nitrite converted to nitrate by nitrite-oxidising bacteria, during which N_2O can be produced by nitrifier denitrification by AOB or by chemical reactions of biological intermediates (Kampschreur et al. 2009). Biological nitrogen conversions and the points at which N_2O can be produced are illustrated in Figure 2.1.

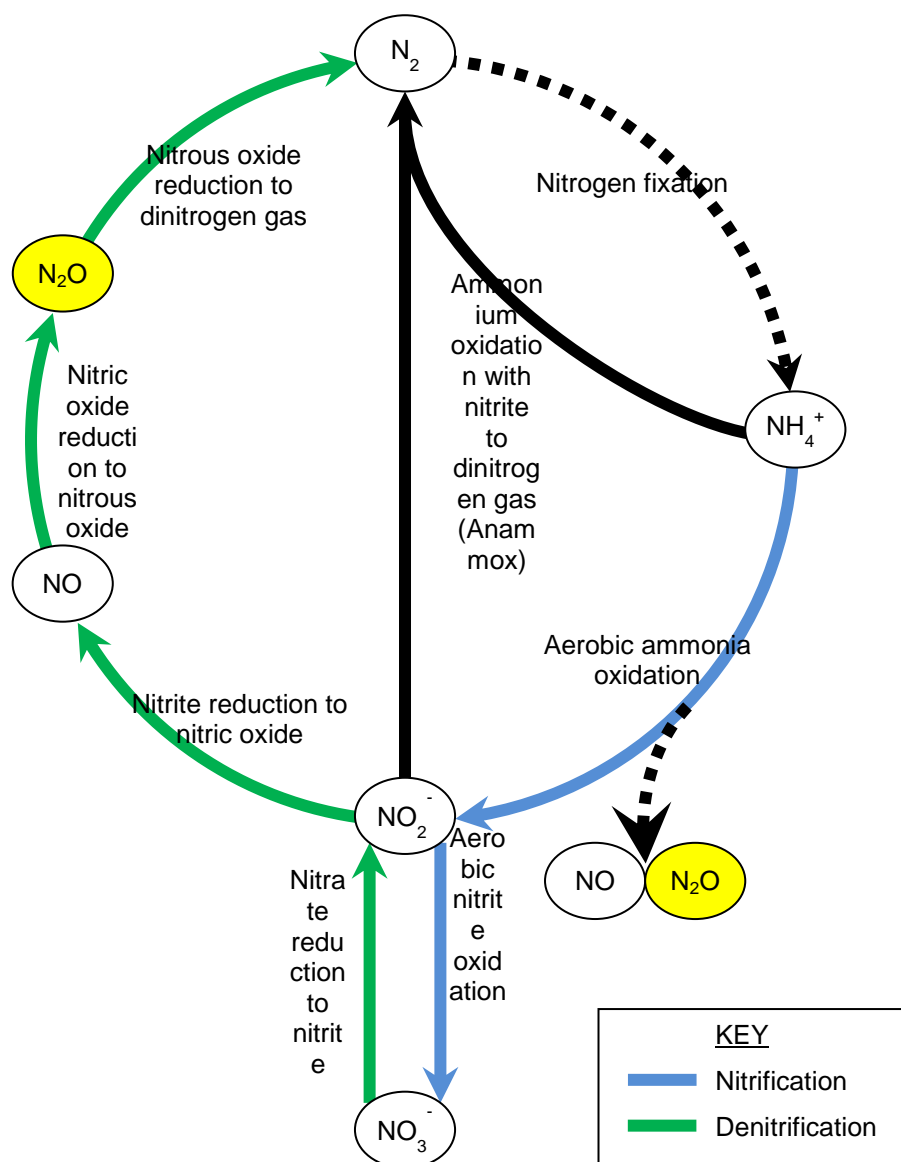


Figure 2.1: Biological nitrogen conversions (adapted from Kampschreur et al. 2009)

Knowledge regarding quantification of N_2O emissions during wastewater treatment is less complete than that of CO_2 and CH_4 . There have been recent investigations into the factors influencing N_2O emissions (e.g. Tallec et al. 2008, Kampschreur et al. 2009, Foley et al. 2010, Rassamee et al. 2011), but there is

no consensus on a method which can be used to estimate emissions with any degree of certainty.

Kampschreur et al. (2009) reported that N_2O is produced predominantly in activated sludge units, as a result of nitrification and incomplete denitrification. Although it may be produced in both the anoxic and aerated stages, the majority will be emitted from aerated compartments. If oxygen is present for nitrification or nitrite for denitrification, additional N_2O may be emitted during grit removal, pre-sedimentation, secondary clarification, sludge storage and anaerobic sludge digestion. UKWIR (2005, quoted in Georges et al. 2009) suggested that N_2O emissions during secondary treatment can be considered to be 0.004 times the nitrogen load, although in reality it is dependent on the amount of nitrification that the plant achieves.

When relating N_2O generation to the mass of nitrogen denitrified, generation factors are still highly variable and cannot reliably be used to estimate emissions. Foley et al. (2010), for example, calculated generation factors in the range of 0.006 - 0.253 kg N_2O -N/kg N denitrified for seven WWTPs studied.

The 2006 IPCC Guidelines for National Greenhouse Gas Inventories proposed an emission factor of 3.2 g N_2O /year per capita for WWTPs with controlled nitrification and denitrification steps (IPCC 2006b). However it has been shown that N_2O generation is affected by process conditions such as DO concentration and COD/N ratio (Kampschreur et al., 2009) and varies considerably between WWTPs. As such, using a per capita emission factor to compare N_2O emissions resulting from different management strategies would be inappropriate.

Kampschreur et al. (2009) found that factors affecting N_2O emissions include the following:

1. Dissolved oxygen: Low DO concentrations during nitrification, resulting from insufficient aeration and/or high organic loading, lead to higher N_2O emissions. However during denitrification, over aeration and high DO concentrations may increase N_2O emissions.
2. Nitrite: High nitrite concentrations increase N_2O emissions during both nitrification and denitrification stages. High nitrate concentrations may arise due to insufficient aeration, low solids retention time (SRT), low

temperature, high ammonium concentration or presence of toxic compounds.

3. Rapidly changing process conditions: An increase in N₂O emissions following a rapid change in environmental conditions has been observed in lab-scale studies. However the influence on emissions from a larger WWTP is uncertain and there is limited suitable data for assessing the impacts.
4. COD/N ratio: During denitrification, low COD (due to influent characteristics or overly efficient pre-sedimentation) results in an increase in N₂O emissions.
5. Consumption of internal storage compounds: denitrification by glycogen accumulating organisms results in greater N₂O emissions.
6. pH: Previous studies have shown that pH affects production of N₂O, but the results do not provide a consensus on the relationship observed. However given that the pH in WWTPs is generally stable, the effect is expected to be minimal.

The most significant operational parameters when attempting to reduce N₂O emissions from WWTPs were identified as: ensuring a sufficiently high DO concentration during the nitrification stage; reducing nitrite concentrations during both nitrification and denitrification; and maintaining a suitably high COD/N ratio during denitrification (Kampschreur et al. 2009). However no quantitative relationships between the process variables and N₂O emissions were derived.

In batch experiments, Tallec et al. (2008) found N₂O emissions from denitrification to be relatively low under anaerobic conditions ($12.6 \pm 27\% \mu\text{g N}_2\text{O-N/g SS/h}$), increasing significantly to $49.7 \pm 9\% \mu\text{g N}_2\text{O-N/g SS/h}$ when the DO concentration increased to 0.3 mg O₂/L and then dropping as oxygen concentration increased further. However whilst these results provide a means of estimating N₂O emissions based on process parameters, they could not be used with any degree of certainty due to the large variability in the results ($\pm 85\%$ with a DO concentration of 2.2 mg/L for example).

Foley et al. (2010) constructed mass balance equations for COD, total nitrogen and liquid phase N₂O across all wastewater treatment processes in order to

calculate the N_2O and total mass of nitrogen emitted to the atmosphere following denitrification. However the mass balance equations used assume steady state, with no net nitrogen accumulation. Whilst this is a reasonable assumption when only analysing emissions over two days in a WWTP with a long SRT, it would not be valid for dynamic modelling over a long time period to evaluate control strategies

2.1.2 Indirect Emissions

Energy Consumption

Emissions resulting from power generation depend on the source of the electricity. Coal, oil, natural gas and renewable sources, for example, will all result in different GHG emissions, for which fixed emission factors ($\text{g CO}_2\text{e/kWh}$) may be used. In order to calculate emissions resulting from energy use at the WWTP, it is therefore necessary to know the source(s) of electricity supplied to the plant. For simplicity, this is sometimes assumed to be the same as the national average electricity generation fuel mix (e.g. Sahely et al. 2006), and generic imported electricity emission factors which take into account the typical UK fuel mix have been published by Defra (2011). However, if a significant proportion of the electricity is from renewable sources then this method will overestimate emissions. Further error may result from variation in emissions from electricity generation between peak and off-peak periods, since plants may operate more (or less) efficiently when required to meet higher demand, and additional power plants using a different energy mix may be bought online during peak periods (Weigel et al. 2010).

The list of equipment requiring electrical energy is extensive; however, when estimating energy consumption in order to calculate indirect GHG emissions from offsite power generation, it is common to consider only the most energy intensive operations (e.g. Cakir and Stenstrom 2005, Shahabadi et al. 2010, Flores-Alsina et al. 2011).

Some previous studies and estimation methodologies for energy requirements have used a ratio of average electricity consumption to volume of water treated to estimate energy use from individual sites (Sahely et al. 2006, Shahabadi et al. 2009, Furubayashi and Nakata 2011); however the energy requirements will evidently differ vastly between sites depending on the processes used, their

size and their operating procedures. Metcalf and Eddy (1994), for example, stated that power requirements for a completely mixed flow regime with mechanical aerators typically vary from 20 - 40 kW/10³ m³ and the precise energy consumption will depend on tank geometry, type and design of the aerator, the temperature and the nature and concentration of suspended solids.

More thorough investigations (e.g. Shahabadi et al. 2010, Flores-Alsina et al. 2011, Gori et al. 2011) have calculated emissions associated with the different processes separately, based on their individual electricity consumption. This approach would be necessary when evaluating control strategies as it would enable, for example, the trade-off between reduced energy consumption and treatment efficiency resulting from reduced aeration to be analysed.

When calculating GHG generation resulting from aerobic wastewater treatment, Cakir and Stenstrom (2005) assumed that electricity demand for aeration is linearly related to oxygen requirements of the aerobic reactor, and used an aeration efficiency of 2 kg O₂/kWh (equivalent to 7.2 g O₂/kJ). However no reasoning behind the choice of efficiency value was given. Despite this, it has been adopted in later research assessing the impact of process design on GHG generation (Shahabadi et al. 2009).

Metcalf and Eddy provided Eq. 2.15 to calculate the power required for adiabatic compression and stated that this can be used for blowers in preliminary treatment, primary treatment and secondary treatment. However, whilst use of this equation should provide a more accurate indication of power consumption than the aforementioned aeration efficiency, it requires detailed process information which may not be available.

$$P_w = \frac{wRT_1}{29.7ne} \left[\left(\frac{p_2}{p_1} \right)^{0.283} - 1 \right] \text{ (SI units)} \quad \text{Eq. 2.15}$$

where:

- P_w = power requirement of each blower [kW]
- w = weight of flow of air [kg/s]
- R = engineering gas constant for air, 8.314 kJ/kmol K
- T_1 = absolute inlet temperature [K]
- p_1 = absolute inlet pressure [atm]
- p_2 = absolute outlet pressure [atm]

- $n = (k-1)/k = 0.283$ for air
- $k = 1.395$ for air
- 29.7 = constant for SI units conversion
- $e =$ efficiency (normal range for compressors is 0.70 to 0.90)

Energy for mixing is required at several stages during wastewater treatment. For flocculation, a range of different types of mixers can be used; paddle mixers, for example, consist of a series of paddles mounted on a vertical or horizontal shaft and driven by a variable-speed drive. The power required to drive a paddle system is related to the drag force on the paddles, as defined in Eq. 2.16 (Metcalf and Eddy 1994):

$$P = F_D v_P = \frac{C_D A \rho v_p^3}{2} \quad \text{Eq. 2.16}$$

where:

- $P =$ power requirement [W]
- $F_D =$ drag force [N]
- $C_D =$ coefficient of drag of a paddle moving perpendicular to fluid
- $A =$ cross- sectional area of paddles [m^2]
- $\rho =$ mass density of fluid [kg/m^3]
- $v_p =$ relative velocity of paddles with respect to the fluid [m/s], usually assumed to be 0.6 to 0.75 times the paddle tip speed

For turbine and propeller type flocculators, which consist of a vertical shaft with three or four blades, the power requirement can be estimated using Eq. 2.17 (Metcalf and Eddy 1994):

$$P = N_P \rho n^3 D^5 \quad \text{Eq. 2.17}$$

where:

- $P =$ power requirement [W]
- $N_P =$ power number for impeller [-]
- $\rho =$ density [kg/m^3]
- $n =$ revolutions per second [r/s]
- $D =$ diameter of impeller [m]

However, use of Eq. 2.16 and Eq. 2.17 again requires detailed knowledge of process variables which may not be available when assessing the overall GHG emissions from the plant and analysing control strategies. Simpler estimations

can be made based upon the volume of the processing unit; Metcalf and Eddy (1994) provide the following typical energy requirements for different stages of treatment:

- Mechanical mixing in the anoxic zone typically requires 0.008 - 0.013 kW/m³ of reactor volume.
- Mixing of flow equalisation basins to prevent the deposition of solids typically requires 0.004 - 0.008 kW/m³ of storage for medium strength wastewater with a suspended solids concentration of approximately 210 mg/l.
- Mechanical anaerobic digester mixing systems have a typical power requirement of 0.005 - 0.008 kW/m³ of digester volume.

Embodied Carbon

GHG emissions from the extraction and processing of materials imported and used in wastewater treatment can be significant (e.g. Shahabadi et al. 2009). These primarily include alkalinity used to control pH and methanol used to provide an external carbon source, although other additives may include polymers, coagulants etc.

Embodied carbon associated with onsite chemical usage is typically estimated using a simple emission factor. Shahabadi et al. (2010), for example, used emission factors of 1.74 g CO₂/g and 1.54 g CO₂/g MeOH for the production and transmission of alkalinity (unspecified source) and methanol respectively. Given that WWTP control strategies will not affect processes used for chemical manufacture or the distance over which they are transported, it is reasonable to assume fixed emissions per unit mass of added chemicals during dynamic modelling and control strategy optimisation.

Reactor Effluent

Research by Cakir and Stenstrom (2005) identified dissolved CH₄ in effluent as a potentially significant contributor to overall GHG emissions, particularly following anaerobic treatment of low strength wastewaters. Although CH₄ concentrations in anaerobic digester effluent are low, the mass in effluent from anaerobic wastewater treatment can be equivalent to the CH₄ in the recovered biogas. Based on this observation, some recent studies (Shahabadi et al. 2009,

Shahabadi et al. 2010) have also considered the effects of dissolved CH₄ when estimating total GHG emissions arising from wastewater treatment. Cakir and Stenstrom (2005) calculated the dissolved CH₄ in effluent from anaerobic processes using Henry's Law and the partial pressure of CH₄ in the reactor, as shown in Eq. 2.18:

$$T_{CH_4}^{AR, Eff} = \frac{Q \times K_{HCH_4}^{AR} \times Pr_{CH_4}^{AR}}{1000} \quad \text{Eq. 2.18}$$

where

$$\begin{aligned} T_{CH_4}^{AR, Eff} &= \text{CH}_4 \text{ production from anaerobic reactor effluent [kg/d]} \\ Q &= \text{wastewater flow rate [m}^3\text{/d]} \\ K_{HCH_4}^{AR} &= \text{Henry's Law constant for CH}_4 \text{ in anaerobic reactor} \\ &\quad \text{[mg/L.atm]} \\ Pr_{CH_4}^{AR} &= \text{partial pressure of gas in reactor [atm]} \end{aligned}$$

Accurate application of this method is dependent on knowledge of temperatures in the reactor and digester (to determine Henry's Law constants) and partial pressures; any assumptions required would increase uncertainty in emission estimates.

Degradation of biosolids remaining in the effluent under anaerobic conditions will result in the formation of CO₂ and CH₄. Many studies (e.g. Keller and Hartley 2003, Cakir and Stenstrom 2005, Greenfield and Batstone 2005, Monteith et al. 2005) have not included the effect of biological processes occurring offsite in their estimation of GHG emissions associated with waste water treatment, however Shahabadi et al. (2009) have shown that offsite emissions can contribute to over 30% of the total emissions from biological processes.

Further emissions due to degradation of remaining BOD in wastewater by biological processes have also been included in few past estimation methodologies. Shahabadi et al. (2010) calculated offsite CO₂ generation from effluent as for onsite aerobic biodegradation, based on the stoichiometry and the known effluent BOD concentration (as detailed in Section 2.1.1). However, no justification is given for the assumption that conditions are aerobic; should oxygen be limited then CH₄ may be formed, greatly increasing the GWP of emissions.

N₂O emissions from receiving waters also occur, as a result of further nitrification and denitrification (e.g. Préndez and Lara-González 2008, Kampschreur et al. 2009). According to the IPCC (2006b), indirect N₂O emissions from wastewater effluent are much more significant than direct N₂O emissions. They provide a simple methodology for their estimation (Eq. 2.19 and Eq. 2.20), using a per capita protein consumption and default emission factor of 0.005 kg N₂O-N/kg N (equivalent to 0.0079 kg N₂O/kg N). This is based on the assumption that all nitrogen is discharged with the effluent; if emissions from controlled nitrification and denitrification in the plant are calculated, then the mass of nitrogen associated with this must be subtracted from the per capita total used to calculate emissions from the effluent.

$$N_2O \text{ emissions} = N_{EFFLUENT} \times EF_{EFFLUENT} \times 44/28 \quad \text{Eq. 2.19}$$

where:

$$\begin{aligned} N_2O \text{ emissions} &= \text{N}_2\text{O emissions in inventory year [kg N}_2\text{O/yr]} \\ N_{EFFLUENT} &= \text{Nitrogen in effluent discharged to aquatic environments [kg N/yr], estimated using Eq. 2.20} \\ EF_{EFFLUENT} &= \text{Emission factor for N}_2\text{O emissions from discharged wastewater [kg N}_2\text{O-N/kg N]} \\ 44/28 &= \text{Conversion of kg N}_2\text{O-N into kg N}_2\text{O} \end{aligned}$$

$$N_{EFFLUENT} = (P \times Protein \times F_{NPR} \times F_{NON-CON} \times F_{IND-COM}) - N_{SLUDGE} \quad \text{Eq. 2.20}$$

$$\begin{aligned} P &= \text{population} \\ Protein &= \text{annual per capita protein consumption [kg/person/yr]} \\ F_{NPR} &= \text{Fraction of nitrogen in protein, default = 0.16 [kg N/kg protein]} \\ F_{NON-CON} &= \text{Factor for non-consumed protein added to the wastewater, default = 1.4 for developed countries} \\ F_{IND-COM} &= \text{Factor for industrial and commercial co-discharged protein in the sewer system, default = 1.25} \\ N_{SLUDGE} &= \text{Nitrogen removed with sludge, default = 0 [kg N/yr]} \end{aligned}$$

Whilst this method could be used in dynamic modelling and evaluation of control strategies, it assumes that N₂O production in aquatic environments is related directly to the total nitrogen discharged into them and makes no allowance for different forms of nitrogen present in the effluent or different combinations of nitrogen conversions that may occur. The emission factor also has a large associated uncertainty (IPCC 2006b).

Solid Waste Disposal

Disposal of sludge may contribute to indirect GHG emissions. Disposal methods typically include landfill, incineration or application to land, all of which have associated emissions. Incineration of sludge results in emissions of CO₂, N₂O and CH₄, although CH₄ emissions are likely to be insignificant (IPCC 2000). When sludge is landfilled or applied to land as fertiliser, further degradation occurs. If this degradation occurs under anaerobic conditions then CO₂ and CH₄ are produced (Shahabadi et al. 2009). Transport of waste from the WWTP to the disposal site contributes further CO₂ emissions (Flores-Alsina et al. 2011).

Emissions resulting from the transportation of waste from the WWTP to disposal site have been considered in few methodologies. Defra (2011) provided a set of CO₂ conversion factors for direct emissions from road freight for use in company reporting, but application of these to wastewater treatment would require a detailed knowledge of trucking movements. To address this problem, Flores-Alsina et al. (2011) used assumed distances to each disposal site and distributed waste between each in fixed proportions. Whilst this may not be an entirely accurate representation, a more detailed analysis would not be possible without detailed site-specific data; this method could provide a reasonable indication of emissions associated with the transportation of waste when developing strategies for the reduction of GHG emissions.

Stripping of CH₄ dissolved in anaerobic digester effluent was identified as another contributor to GHG emissions by Cakir and Stenstrom (2005), who calculated the dissolved CH₄ using Eq. 2.21, based upon Henry's Law and the partial pressure of CH₄ in the digester (as for the reactor effluent).

$$T_{CH_4}^{D_Eff} = \frac{P \times K_{HCH_4}^D \times Pr_{CH_4}^{AD}}{1000} \quad \text{Eq. 2.21}$$

where

$$\begin{aligned}
T_{CH_4}^{D_Eff} &= \text{CH}_4 \text{ production from anaerobic digester effluent [kg/d]} \\
P &= \text{sludge flow rate [m}^3\text{/d]} \\
K_{HCH_4}^D &= \text{Henry's Law constant for CH}_4 \text{ in anaerobic digester} \\
&\quad \text{[mg/L.atm]} \\
Pr_{CH_4}^{AD} &= \text{partial pressure of gas in digester [atm]}
\end{aligned}$$

However, they noted that the impact of CH₄ dissolved in anaerobic digester effluent is generally small due to the low flows of concentrated biosolids. As such, more recent estimation methodologies which accounted for dissolved CH₄ (Shahabadi et al. 2010) only included CH₄ in the anaerobic reactor effluent.

A number of different approaches have been taken to estimating emissions from degradation of sludge when landfilled or applied to land as fertiliser. Flores-Alsina et al. (2011) calculated CO₂ emissions from mineralisation using a CO₂ to carbon factor and carbon concentration of the sludge. However Shahabadi et al. (2009) noted that sludge disposal can result in emissions of CH₄ in addition to CO₂ under anaerobic conditions; omission of CH₄ production could have a significant effect on the overall CO₂e emission estimate due to its relatively high GWP. Shahabadi et al. (2009) assumed that degradation occurs under anaerobic conditions in accordance with Eq. 2.4. Based on stoichiometry, CH₄ and CO₂ emissions resulting from biomass decay were then calculated using Eq. 2.22 and Eq. 2.23; however use of this method assumes that all biosolids in the effluent will degrade. No allowance was made for the effects of BOD utilisation.

$$M_{CO_2, SludgeDegradation} = 0.58 \times P_{DegradableSSeffSludge}^D \quad \text{Eq. 2.22}$$

$$M_{CH_4, SludgeDegradation} = 0.35 \times P_{DegradableSSeffSludge}^D \quad \text{Eq. 2.23}$$

where:

$$\begin{aligned}
M_{CO_2, SludgeDegradation} &= \text{rate of CO}_2 \text{ production [g CO}_2\text{/day]} \\
M_{CH_4, SludgeDegradation} &= \text{rate of CH}_4 \text{ production [g CH}_4\text{/day]} \\
P_{DegradableSSeffSludge}^D &= \text{biodegradable solids in digester effluent [g/day]}
\end{aligned}$$

Application of sludge to land can also result in N₂O emissions. The IPCC (2006a) recommend an emission factor of 0.01 kg N₂O-N/kg N for sludge applied to managed soils.

Sludge may alternatively be incinerated. The IPCC (2000) recommend that CO₂ and N₂O emissions from sludge incineration are calculated using Eq. 2.24 and Eq. 2.25 respectively, both of which utilise an emission factor.

$$\text{CO}_2 \text{ emissions [Gg/yr]} = IW \times CCW \times FCF \times EF_{\text{CO}_2} \times 44/12 \quad \text{Eq. 2.24}$$

$$\text{N}_2\text{O emissions [Gg/yr]} = IW \times EF_{\text{N}_2\text{O}} \times 10^{-6} \quad \text{Eq. 2.25}$$

where:

CCW = fraction of carbon content in sewage sludge

FCF = fraction of fossil carbon in sewage sludge

EF_{CO2} = burn out efficiency of combustion of incinerators for sewage sludge

44/12 = conversion from C to CO₂

EF_{N2O} = aggregate N₂O emission factor for sewage sludge [kg N₂O/Gg]

IW = amount of incinerated sewage sludge [Gg dry weight/yr]

CO₂ emissions are calculated using the fossil carbon content, total carbon content and burn out efficiency during combustion, for which default values are provided. If country-specific data is unavailable, then the following values are recommended: *CCW* = 30%, *FCF* = 0% and *EF_{CO2}* = 95% (IPCC 2000).

The default value provided of 0% fossil carbon content in sewage sludge is based on the assumption that emissions resulting from incineration of the carbon fraction derived from biomass materials should not be included in emissions estimates, and their use suggests that incineration of sludge results in no CO₂ emissions. This is clearly not the case and when attempting to develop carbon management strategies it is essential that all sources of CO₂ are accounted for. Furthermore, the use of a fixed burn out efficiency makes no allowance for the effects that changing sludge compositions or process conditions may have on the completeness of combustion and suggests that emissions can be reduced simply by decreasing the burn out efficiency. The method could be modified to include emissions from incineration of biomass materials, which would enable a basic estimate of CO₂ emissions from incineration of sludge to be made; however, a more detailed method would be preferable for the assessment of control strategies.

Use of Eq. 2.25 for estimation of N_2O emissions from sludge incineration is very basic, using only an aggregate emission factor per unit weight of sludge. Default emission factors are provided: for fluidised bed incineration plants in the UK, these typically range from 100 - 1500 kg N_2O /Gg sewage sludge (dry matter). This method does not make allowance for variations in nitrogen content of the sludge (unless different emission factors are calculated and used accordingly) and would therefore be unsuitable for dynamic modelling of systems and optimisation of process control to reduce emissions; only reducing the mass of sludge produced would lower emissions using this estimation method.

2.2 Modelling Greenhouse Gas Emissions from Wastewater Treatment

This section of the literature review aims to analyse and assess existing emission estimation models with respect to their suitability for dynamic modelling of WWTPs for assessment of GHG emissions and development of real time control strategies.

2.2.1 Scope of Existing Emission Estimation Models

Following advances in GHG estimation techniques, a number of models have been developed for estimating GHG emissions from WWTPs and five of the most comprehensive (as of April 2012; more recent developments are discussed in Section 2.2.8) are analysed in this chapter. The main differences in the WWTPs modelled were due to the reactor design. All models used an anaerobic digester; none included aerobic digestion. The key features of the layouts modelled are as follows:

- Cakir and Stenstrom (2005) modelled both an anaerobic WWTP (with an anaerobic reactor and anaerobic digester) and an aerobic treatment plant (with an aerobic reactor and anaerobic digester) to enable a comparison of emissions from the two setups.
- Préndez and Lara-González (2008) utilised a range of existing models to estimate GHG emissions resulting from different components of the wastewater system, including both anaerobic and aerobic reactors.
- Shahabadi et al. (2010) considered a hybrid treatment system, with an anaerobic reactor followed by an anoxic/aerobic reactor.

- Flores-Alsina et al. (2011) adapted the IWA BSM2, and therefore used the same plant layout, which included an activated sludge reactor. The new model is referred to as BSM2G.
- Gori et al. (2011) used an activated sludge reactor.

The emissions accounted for in each of the aforementioned, recently published models are detailed in Table 2.2 to enable a comparison of different modelling approaches and the limitations of each. Emissions which were estimated using empirical relationships are identified, as they may produce results of questionable reliability if applied to systems with an unusual set up, and may not behave as predicted when control strategies are applied.

Table 2.2: Comparison of models previously used for estimation of GHG emissions from WWTPs

Source of emissions		Cakir and Stenstrom (2005)	Prédez and Lara-González (2008)	Shahabadi et al. (2010)	Flores-Alsina et al. (2011)	Gori et al. (2011)
Direct emissions	<u>Methane</u>					
	Stripping of dissolved CH ₄ formed in sewer system	x	x	x	x	x
	Poorly managed aerobic treatment	x	x	x	x	x
	Anaerobic reactor	✓T	✓E	✓T	x	x
	Anaerobic digester	✓T	✓T	✓T	✓T	✓T
	Biogas leakage	x	x	✓?	x	✓E
	Biosolids dewatering	x	x	x	x	✓E
	<u>Carbon dioxide</u>					
	Aerobic reactor	✓T	x	✓T	✓T	✓T
	Anaerobic reactor	✓E	✓?	✓T	x	x
	Aerobic digester	x	✓?	x	x	x
	Anaerobic digester	✓E	✓?	✓T	✓T	✓E
	Biogas leakage	x	x	✓?	x	✓E
	Biogas combustion	✓E	x	✓T	✓T	✓T
	<u>Nitrous oxide</u>					
	Nitrification and/or denitrification in wastewater treatment	x	✓E	x	✓T	x
	Nitrification and/or denitrification in sludge treatment	x	✓E	x	x	x
Indirect emissions	<u>Energy consumption</u>					
	Generic energy consumption / other equipment	x	✓E	✓E	x	✓E
	Pumping	x	x	x	✓E	✓E
	Aeration	✓E	x	✓E	✓E	✓E
	Heating	✓E	x	✓T	✓E	✓E
	Mixing	x	x	x	✓E	x
	<u>Embodied carbon</u>					
	Chemicals	x	x	✓E	✓E	x
	<u>Reactor effluent</u>					
	Stripping of dissolved CH ₄	✓T	x	✓T	x	x
	Degradation of remaining biosolids	x	x	✓?	x	x
	Nitrification and denitrification	x	x	x	x	x
	<u>Digester effluent</u>					
	Transportation	x	x	✓E	✓E	x
	Stripping of dissolved CH ₄	✓T	x	x	x	x
	CH ₄ from degradation	x	✓E	✓T	x	x
	CO ₂ from degradation	x	✓E	✓T	✓E	x
	N ₂ O from nitrogen conversion	x	✓E	x	x	x

KEY: ✓E = Empirical method, ✓T = Method with theoretical basis,
✓? = Method not detailed, x = Not calculated

2.2.2 Modelling of Direct Emissions

It can be seen from Table 2.2 that the choice of direct emission sources for inclusion in each model was similar. All included emissions from aerobic reactors, anaerobic digestion and, when part of the WWTP layout, anaerobic reactors. However emissions resulting from unintentionally anaerobic conditions and the stripping of CH_4 formed in the sewers were not considered and only one model included emissions from the biosolids dewatering unit.

Anoxic/Aerobic Reactors

Using aerobic wastewater treatment processes inhibits CH_4 production, although GHGs are not eliminated as CO_2 and N_2O are still produced. All WWTPs modelled incorporated aerobic reactors, but the extent to which their direct emissions were included varied; N_2O formation, for example, was only included only by Préndez and Lara-González (2008) and Flores-Alsina et al. (2011) due to the complexity of nitrogen conversion processes.

According to the IPCC (2006b), CO_2 emissions from wastewater should not be considered in GHG inventories as they are of biogenic origin. As such, Préndez and Lara-González (2008) did not include CO_2 emissions from the aerobic reactor. However in order to develop a comprehensive model of GHG emissions resulting from wastewater treatment for the development of carbon management strategies, it is necessary to include all potential sources.

Cakir and Stenstrom (2005) related CO_2 emissions to BOD reduction only, utilising a yield factor $1.375 \text{ kg CO}_2/\text{kg BODu}$ for the activated sludge process. The origin of this factor was not detailed, and it differs significantly from those used in other models and estimation methodologies. Shahabadi et al. (2010) and Flores-Alsina et al. (2011) provided a more detailed methodology, attributing CO_2 emissions to a number of different processes occurring within the reactor and using stoichiometry to derive theoretical emission factors. However each used different formulae to represent utilisation of carbonaceous BOD and biomass decay, therefore resulting in significantly different emission factors: $0.33 \text{ g CO}_2/\text{g COD}$ and $1.56 \text{ g CO}_2/\text{g VSS}$ for Shahabadi et al. (2010) and $1.1 \text{ g CO}_2/\text{g O}_2$ (equivalent to $1.1 \text{ g CO}_2/\text{g COD}$) and $1.95 \text{ g CO}_2/\text{g VSS}$ for Flores-Alsina et al. (2011).

Shahabadi et al. (2010) also included CO₂ emissions resulting from nutrient removal activities to improve the completeness of the model. They assumed that nitrogen removal is carried out by the nitrification-denitrification process and used stoichiometric relationships to derive emission factors of 2.62 g CO₂/g N-nitrate and 2.81 g CO₂/g N-nitrate for denitrification with and without an external carbon source respectively.

The model developed by Flores-Alsina et al. (2011) made allowance for CO₂ utilisation during nitrification, applying this as CO₂ credit. CO₂ credit was calculated using an emission factor of 0.31 g CO₂/g N nitrified.

Nutrient removal activities can also result in emissions of N₂O from the reactors. Préndez and Lara-González (2008) included GHG emissions from incomplete nitrification and denitrification in their model, but the method was based upon the use of activity data (e.g. population served) and empirical emission factors, and would therefore be unsuitable for use in control strategy optimisation. Flores-Alsina et al. (2011) included N₂O emissions from heterotrophic denitrification in the water line, as calculated by the modified Activated Sludge Model for Nitrogen (ASMN), but did not consider emissions associated with nitrification.

Anaerobic Reactor

Emissions from anaerobic reactors, where modelled, were typically estimated using emission factors. Préndez and Lara-González (2008) again utilised activity data and empirical emission factors and their model might, therefore, produce results of questionable reliability if used in the development of control strategies.

The model of Cakir and Stenstrom (2005) offered some improvement, in that they utilised the modelled reaction kinetics and made allowance for some of the CH₄ produced entering solution in accordance with Henry's Law. However, they only considered CH₄ and CO₂ production associated with BOD reduction using emission factors of 0.25 g CH₄/g BOD_u and 0.69 g CO₂/g BOD_u, respectively, for which no explanation was given. The CO₂ emission factor differs significantly from that given by Shahabadi et al. (2010) of 0.27 g CO₂/g BOD, which was derived from stoichiometry (Eq. 2.3), and might therefore provide an overestimate. The CH₄ emission factor used in both models is of questionable

reliability, as the stoichiometric relationship provided yields a factor of 0.25 g CH₄/g COD (not BOD).

Shahabadi et al. (2010) offered further improvement by including biomass decay as a contributing factor to emissions from the anaerobic reactor. Emission factors of 0.35 g CH₄/g VSS and 0.58 g CO₂/g VSS were used, based on the theoretical reaction equation provided (Eq. 2.4).

Anaerobic Digester

Production of CO₂ and CH₄ in the anaerobic digester was included in all of the models compared, using a range of different methods. As for the anaerobic reactor, Cakir and Stenstrom (2005) included only emissions resulting from BOD oxidation, using the theoretical CH₄ yield factor for COD reduction to estimate emissions due to BOD reduction. Allowance was made for CH₄ dissolved in the digester effluent (calculated using Henry's Law) when estimating the biogas composition.

Shahabadi et al. (2010) stated that their method for estimating emissions from the anaerobic digester was similar to that for the anaerobic reactor, which included calculation of GHG production during BOD reduction and biomass decay using theoretical emission factors; however the differences were not explained beyond the fact that it was assumed 70% of the available biomass in the digester degraded.

The existing Anaerobic Digestion Model No.1 (ADM1, as incorporated in BSM2) was used by Flores-Alsina et al. (2011) to calculate both CH₄ and CO₂ emissions from anaerobic digestion.

Gori et al. (2011) calculated CH₄ production in the anaerobic digester due to COD oxidation only, using a theoretical emission factor of 0.35 Nm³ CH₄/kg biodegradable COD, derived from stoichiometry (Eq. 2.3). CO₂ production was estimated empirically, based on the calculated CH₄ production and an assumption that this constitutes a fixed proportion of the biogas; this method makes no allowance for changing biogas composition resulting from different operational parameters.

Préndez and Lara-González (2008) also modelled N₂O emissions resulting from incomplete nitrification and denitrification during sludge treatment. However, as

for the reactor, the calculation used activity data and empirical emission factors and would therefore be unsuitable for providing an accurate indication of the effects of adjusting operational procedures.

Biogas Leakage and Combustion

CO₂ emissions from the combustion of biogas were generally included in models, although the technique was not always clear. The method provided by Cakir and Stenstrom (2005), for example, was particularly ambiguous, being based upon the anaerobic reactor and digester oxygen requirement and a CO₂ yield factor in terms of kg CO₂/kg BOD_u. The remaining models used a theoretical emission factor of 2.75 g CO₂/g CH₄, based on stoichiometry (Eq. 2.14), in conjunction with the modelled CH₄ production. This relies on the assumption that all CH₄ is fully combusted. If combustion is incomplete, however, then this will impact on both direct and indirect emissions: direct emissions will have a higher GWP than calculated due to the presence of non-combusted CH₄ and indirect emissions resulting from energy generation will be higher due to a lower offset from energy recovery than calculated.

Some biogas could also be leaked directly to the atmosphere, therefore reducing energy recovery and increasing the GWP of emissions as some CH₄ does not undergo combustion. Allowance for biogas leakage was made by Shahabadi et al. (2010) and Gori et al. (2011), although the latter only included CH₄ emissions, which were assumed to be 2% of the biogas generated. The method used by Shahabadi et al. (2010) for quantifying leaks was not provided.

Biosolids Dewatering

Emissions released during biosolids dewatering were modelled only by Gori et al. (2011) and the method used was not explained in detail. It was assumed that half of the CH₄ contained in the biogas-saturated biosolids was released directly to the atmosphere during dewatering and the rest recirculated and converted to CO₂ during biological oxidation; however it is unclear how the CH₄ content of the biosolids was determined.

2.2.3 Modelling of Indirect Emissions

The inclusion of indirect emissions in models was generally less complete than direct emissions. Préndez and Lara-González (2008), for example, only

included calculation of emissions from the degradation of digester effluent and generic energy consumption.

Energy Consumption

Indirect emissions resulting from energy consumption were modelled in all five of the models compared, based on the generation of power imported and/or the combustion of biogas as a renewable energy source. Calculation of emissions attributed to power generation varied greatly: Cakir and Stenstrom (2005) and Gori et al. (2011), for example, used emission factors of 0.96 kg CO₂e/kWh and 0.245 kg CO₂e/kWh respectively and neither provided any justification for the values chosen. This large variation is not unexpected, as previous studies have used factors within the range 0.21 – 0.77 kg CO₂e/kWh to account for differences in the energy generation mix (Sahely et al. 2006); however it means that the choice of emission factor could have a significant effect on the calculated overall GHG emissions.

A range of methods were used to estimate the energy requirement of the WWTP, although they were generally more comprehensive in later models. Typically only the most energy intensive operations (including pumping, aeration, heating and mixing) were considered (Cakir and Stenstrom 2005, Shahabadi et al. 2010, Flores-Alsina et al. 2011).

When calculating the energy required for aeration, several models utilised empirical formulae to provide a basic estimate; however, the emission factors varied considerably. Cakir and Stenstrom (2005), for example, used a fixed aeration efficiency of 2 kg O₂/kWh, whereas Shahabadi et al. (2010) used a factor of 7.2 g O₂/kJ (equivalent to 25.9 kg O₂/kWh). This large variation suggests that such a method of calculation may not be robust. Furthermore, Shahabadi et al. (2010) calculated aeration energy based on the oxygen demand of the aerobic reactor, therefore making the assumption that the oxygen supplied is equal to the oxygen required. Whilst this method could be used in carbon accounting and control strategy development to provide an indication of likely energy use, accuracy could be improved by taking into account the effect of aeration rate on efficiency. Flores-Alsina et al. (2011) used the aeration energy calculation within the BSM2, which is based upon a more

detailed methodology, valid specifically for Degremont DP230 porous disks at an immersion depth of 4m.

Flores-Alsina et al. (2011) also modelled the energy required for mixing and pumping using the original BSM2 methodology, in which pumping energy is related linearly to the volume of water pumped, using different emission factors for each pumping location. Similarly, Gori et al. (2011) used a fixed specific energy consumption (kWh/m^3) for influent pumping. This method makes no allowance for the maximum pumping capacity and the effect of flow rate on efficiency.

When modelling the energy required for heating of the anaerobic digester, Gori et al. (2011) related it only to the mass of sludge treated, using an empirical emission factor of $0.16 \text{ kWh/kg dry solids}$. This implies that power used is linearly related to the mass of sludge treated, which may not be a valid assumption during dynamic modelling if there is temporal variation in influent temperature. Shahabadi et al. (2010) provided a more versatile method for calculating the energy required for heating, based on a specific heat of $4,200 \text{ kJ/kg/}^\circ\text{C}$ for wastewater, the modelled influent temperature and flow rate and the required digester temperature.

Models typically offset the energy requirement of the plant with the energy recovery from CH_4 combustion. Methods used to calculate energy recovery from biogas were similar and typically applied a heat conversion efficiency of 0.83 (Cakir and Stenstrom 2005, Shahabadi et al. 2010) or an electricity generation efficiency of 0.43 (Flores-Alsina et al. 2011) to the theoretical energy content of the CH_4 combusted (50 MJ/kg CH_4). Gori et al. (2011) used the same method, but with a specific energy of $35.8 \text{ MJ/m}^3 \text{ CH}_4$ and an energy recovery efficiency of 0.5. This method provides a straightforward means of estimating energy generation; however given that the density of CH_4 varies with temperature it would be preferable to specify the specific energy of CH_4 in terms of mass, not volume. Furthermore, allowance should be made for instances when the energy demand is less than the energy recovered. Unless the surplus energy is stored in these cases, the average energy offset across the simulation period would be less than the energy recovery calculated based on only the conversion efficiency and theoretical energy content.

Embodied Carbon

Indirect emissions due to the use of chemicals during treatment were included in only two of the models compared. Shahabadi et al. (2010) used emission factors of 1.74 g CO₂/g and 1.54 g CO₂/g for the production and transmission of alkalinity and methanol respectively, having calculated the mass of chemicals used during treatment processes from stoichiometric equations. Flores-Alsina et al. (2011) only considered external carbon source (methanol) addition, for which the same emission factor was used. Whilst these emission factors were both derived empirically, they could be used in dynamic modelling and assessment of control strategies provided that the mass of chemicals used was calculated accurately, as emissions resulting from chemical production should be unaffected by changes in their end use. Further indirect emissions may result from the use of polymers and coagulants. Embodied carbon should not be overlooked in the development of a comprehensive model, as a previous study (Shahabadi et al. 2009) found that over 50% of total GHG emissions from an anaerobic treatment plant could be attributed to material usage.

Reactor Effluent

Stripping of dissolved CH₄ from the reactor effluent was not commonly included in the models, however where it was assumed that all CH₄ produced was emitted at source (with none entering solution) it would be inappropriate to do so. Cakir and Stenstrom (2005) and Shahabadi et al. (2010) used Henry's Law (Eq. 2.18) and the partial pressure of CH₄ in the anaerobic reactor gas to estimate the mass of CH₄ dissolved in the effluent, and then assumed that all dissolved CH₄ would be later stripped to the atmosphere. Modelling the processes of CH₄ being dissolved in the reactor and subsequently stripped from the effluent has no effect on net emissions from the WWTP (as it is assumed that all CH₄ generated is released at some stage, provided that biogas from the reactor is not combusted) and is, therefore, not essential when calculating total emissions; however, it would be of significance if a distinction between direct and indirect emissions is required.

Digester Effluent

Stripping of dissolved CH_4 from the digester effluent was included in two models: Cakir and Stenstrom (2005) and Shahabadi et al. (2010) estimated the mass of CH_4 dissolved in the sludge using Henry's Law (Eq. 2.18), as for the anaerobic reactor effluent. The BSM2, as used by Flores-Alsina et al. (2011), includes calculation of the CH_4 in solution in the digester; however, stripping of CH_4 remaining in the effluent was not modelled. Given that biogas from the digester is usually combusted, making allowance for CH_4 dissolved in the effluent could result in an increase in the CO_2e of emissions, as it would not be converted to CO_2 (which has a lower GWP). Furthermore it would reduce the energy recovery from biogas combustion, therefore reducing the energy offset and increasing indirect emissions due to the generation of imported energy.

Transportation of sludge can result in further indirect emissions, although these have been included in few models. Flores-Alsina et al. (2011) used an unspecified emission factor ($\text{kg CO}_2\text{e}/\text{mile}/\text{tonne sludge}$). An emission factor of this form could reasonably be used during dynamic modelling of systems as, within the context of developing WWTP control strategies, no changes could be made which would affect the transport efficiency.

Indirect emissions from the degradation of digester effluent have been included, to varying extents, in emission estimation models. Shahabadi et al. (2010), for example, assumed that biomass in the digester effluent degrades anaerobically downstream, although did not specify whether this was modelled in accordance with the stoichiometric relationship used previously to represent biodegradation of biomass in the anaerobic digester or by other means. N_2O emissions from the degradation of sludge were generally omitted; Préndez and Lara-González (2008) identified sludge disposal to landfill or agricultural use as a source of N_2O emissions, but their referenced methodology for calculating emissions only included N_2O from sludge incineration. Where included, indirect N_2O emission models were based on empirical formulae; this could be attributed to the complexity of nitrogen conversion processes and lack of simple models. Whilst models with a theoretical basis would be preferable for the modelling of dynamic systems and assessment of control strategies, an empirical formula relating indirect N_2O emissions to the nitrogen content of the effluent could be

used as offsite processes would be independent of the WWTP operational procedure.

2.2.4 Model Calibration and Verification

GHG emission estimates from the five models analysed were uncalibrated, despite some models being applied to real WWTPs and using measured process parameters. Préndez and Lara-González (2008) incorporated a range of existing models, modified to fit the national conditions and specific scenarios, but did not test the validity of these modifications with real data. This could be attributed partly to a lack of data and difficulties in obtaining a comprehensive set of measurements – particularly for indirect emissions.

Some attempts were made to validate calculated emissions using previously published values. For example, the relationship between the gas phase percentages of biogas constituents and influent substrate concentration modelled by Cakir and Stenstrom (2005) were plotted and compared with a plot of compositions reported in literature. However, whilst similar trends were observed, the magnitude varied considerably; for instance an influent substrate concentration of 10,000 mg COD/L yielded modelled gas phase percentages of 54% CH₄ and 42% CO₂, whereas previously published studies reported compositions in the region of 76% CH₄ and 19% CO₂. As such, there could be significant error in the modelled CH₄ production and subsequent energy recovery.

Emission estimates modelled by Shahabadi et al. (2010) were compared with those obtained in two previous studies, using the same process parameters, in order to obtain an indication of their validity. It was found that the emissions per unit volume of wastewater treated were similar to those reported by Monteith et al. (2005), who used data from an activated sludge plant for calibration. However the calibration data was very limited in terms of GHG production, containing only the total volume of gas produced in the anaerobic digester and no details of its CH₄ and CO₂ content. Additionally, when emissions modelled by Shahabadi et al. (2010) were expressed per unit mass of COD removed, results differed considerably from those reported in literature – this was attributed to differences in wastewater composition and the inclusion of offsite GHG emissions.

Flores-Alsina et al. (2011) made no attempt at calibration, with the justification that the purpose of their model was to provide a means of including GHG emissions when assessing overall WWTP performance rather than predicting emissions with complete accuracy. It was argued that the range of estimates obtained when modelling different scenarios were within the range of values presented in two previous publications, however the variation in these values was large (0.34 – 2.2 kg CO₂e/m³ treated wastewater) and individual results for specific scenarios were not compared.

2.2.5 Model Omissions

From Table 2.2 it can be seen that some sources of emissions were omitted from all models. Unaccounted for emissions of CH₄ and N₂O in particular could have a significant impact on the overall GWP. Emissions due to the stripping of CH₄ formed in the sewer system, for example, were not included in the comprehensive emission estimation models but experimental evidence (Guisasola et al. 2008) has shown that CH₄ formation in the sewer system could increase CH₄ emissions from WWTPs by 12 - 100 %. However there is currently a high degree of uncertainty when estimating these emissions. Guisasola et al. (2009) found that there is a high correlation between CH₄ production and hydraulic residence time (HRT) and the pipe area to volume ratio (A/V), with higher CH₄ concentrations corresponding to a long HRT or large A/V ratio; but whilst it was concluded that CH₄ production in sewers may provide a significant contribution to overall GHG emissions from the wastewater system, dissolved CH₄ stripped within the WWTP boundary was not quantified. A model for CH₄ production in sewers has been developed (Chaosakul et al. 2014); however this is empirical and based on parameters such as wastewater temperature and HRT.

Similarly, direct CH₄ emissions resulting from poorly managed treatment and unintentionally anaerobic conditions were not modelled due to a lack of reliable estimation techniques; however they could be significant, as a recent full-scale investigation (Wang et al. 2011) recorded CH₄ emissions at every processing unit in the WWTP. The omission of CH₄ emissions from poorly managed aerobic treatment could affect the validity of results when attempting to optimise control strategies; for example existing emission estimation methods for aerobic processes may suggest that reducing aeration would lower overall emissions

due to a reduction in electricity consumption, however in reality conditions may become anaerobic, therefore resulting in the production of CH₄ and greatly increasing the GWP of emissions. High CH₄ and N₂O emissions associated with operational problems such as sub-optimal operation of biological nitrogen removal and digester foaming have also been observed in field studies (Yoshida et al. 2014).

Calculation of indirect emissions of N₂O was very limited, with no models including formation of N₂O from the reactor effluent. This could be a significant omission, as several authors (IPCC 2006b, Préndez and Lara-González 2008, Kampschreur et al. 2009) have highlighted the importance of N₂O emissions from receiving waters, most commonly attributed to further nitrification and denitrification. Kampschreur et al. (2009) added that stripping of dissolved N₂O formed during treatment is slow due to its relatively high solubility in water and may be completed outside the boundary of the WWTP, therefore contributing to offsite N₂O emissions. This theory is, however, contradicted by Foley et al. (2010), who recorded less than 5 % of N₂O formed in the WWTP dissolved in the effluent and argued that N₂O is quickly stripped to the atmosphere due to its high mass transfer coefficient.

2.2.6 Model Applications

The models detailed above were used to assess the GHG emissions resulting from wastewater treatment under a number of scenarios, including different treatment types (Cakir and Stenstrom 2005, Préndez and Lara-González 2008), variations in influent characteristics (Cakir and Stenstrom 2005, Shahabadi et al. 2010, Gori et al. 2011) and different control strategies (Flores-Alsina et al. 2011).

Préndez and Lara-González (2008) modelled GHG emissions resulting from six scenarios (incorporating varying proportions of biogas reuse and aerobic and anaerobic treatment). During the period in which 100% of wastewater was treated in a WWTP, it was found that the treatment processes and management strategies yielding the lowest emissions (per m³ of water treated) consisted of 90% aerobic and 10% anaerobic wastewater treatment, 100% anaerobic sludge treatment and 75% biogas reuse. This approach is only meaningful when designing new WWTPs or carrying out extensive modifications to the plant

design; if embodied carbon were included in the emission estimation then it is likely that any major structural changes would not be a feasible solution. Furthermore, the investigation had a very limited scope, with only six discrete scenarios modelled and a maximum of 75% biogas reuse considered. Given that the majority of emission sources were modelled using activity data and empirical emission factors, it would not be feasible to use this model for a detailed analysis as results would be of insufficient accuracy.

In order to identify the most efficient treatment process (in terms of GHG production), Cakir and Stenstrom (2005) modelled the effect of influent ultimate BOD on net CO₂e production for anaerobic and aerobic systems with a range of SRTs. From this it was concluded that aerobic treatment results in lower emissions when the influent BOD_u is low, with anaerobic treatment becoming increasingly competitive as influent BOD_u increases and yielding negative net emissions when the influent BOD_u is greater than 800 mg/L. However no assessment of the treatment efficiency or effluent quality was made and ensuring compliance with legislative standards could affect the calculated emissions. Application and optimisation of control strategies could also have a significant impact on the reported relationship between influent BOD_u and net CO₂e production. Furthermore, the results are of questionable reliability as the model was not calibrated and significant differences between the modelled digester gas composition and compositions previously reported in literature were identified.

Shahabadi et al. (2010) also carried out simulations with a range of influent concentrations, both with and without energy recovery from biogas, but undertook a more detailed analysis of the effect of the influent characteristics on emissions from each process. The manufacture and transportation of alkalinity and methanol, for example, were identified as major sources of GHG generation, suggesting that reduction of their use through efficient process control and optimisation has the potential to reduce overall emissions associated with wastewater treatment. Based on a comparison of the relative contribution of each source to overall emissions, a number of strategies to reduce emissions were recommended. However many of these recommendations, such as “increased energy efficiency to reduce electricity needs” and “increased efficiency of the anaerobic digester to produce more

biogas” were vague, with no guidance on how they might be achieved. Additionally the effects of following more specific recommendations, such as operating the anaerobic digester at a lower temperature to reduce energy used for heating, were not modelled to investigate the associated trade-offs and confirm that they had the desired effects.

Gori et al. (2011) gave a more thorough investigation into the effects of soluble and particulate substrate concentrations on the carbon footprint of wastewater treatment processes: a range of pCOD/VSS influent ratios were tested and sensitivity analysis was carried out to determine the relative parameter variation within the range of influent concentrations modelled. It was found that increasing pCOD/VSS had the greatest impact on CO₂e resulting from biogas combustion and leakage, and caused a reduction in CO₂e from activated sludge respiration and biosolids dewatering.

The only testing of WWTP control strategies with respect to GHG emissions was carried out by Flores-Alsina et al. (2011). Three closed loop control strategies (relating to the DO set point, aeration flow and internal recycle flow rate) were simulated and compared with an open loop base case scenario. It was found that control strategies could be implemented to simultaneously reduce GHG emissions by up to 9.6%, reduce operational costs and improve effluent quality. This included a substantial reduction in aeration energy due to the implementation of a DO controller to improve efficiency of the aeration system and prevent nitrite accumulation. A detailed analysis of the relationship between DO set point, SRT and reactor COD/N ratio and the emissions from each processing unit modelled was also carried out. One of the findings from this analysis was that decreasing the SRT results in a reduction in net emissions due to increased CO₂ credit from energy recovery. This supports the modelled results of Cakir and Stenstrom (2005), in which the total CO₂ production from the WWTP more than doubled when the SRT was increased from 10 days to 30 days.

2.2.7 Modelling Challenges

Several of the models analysed were used to assess the impacts of changing influent conditions on GHG emissions. However given that the influent characteristics are (largely) beyond the control of the water companies, this

information would be of minor importance when developing strategies to meet the CRC requirements whilst ensuring compliance with the UWWTD and WFD requirements. It would be desirable to also consider the effects of adjusting the WWTP operational or control strategies. This would enable different approaches to be evaluated with respect to a number of criteria, including overall emissions, effluent quality, legislative compliance and operational cost.

In order to develop control strategies suitable for real life application, a flexible and transferable emission estimation model is required. Calibration is also important to ensure the validity of results, but existing models are poorly calibrated with respect to GHG emissions (if at all) and collecting sufficient data, particularly from indirect sources, is likely to be challenging.

A detailed assessment of GHG emissions would require a comprehensive model, incorporating existing methodologies for estimation of CH₄, CO₂ and N₂O emissions and sources currently omitted, to enable the relative significance of each source to be determined. However despite past investigations, there is currently a lack of reliable estimation techniques for emissions from some sources, including stripping of CH₄ formed in the sewer network and CH₄ formed under unintentionally anaerobic conditions.

In order to assess the suitability of control strategies, dynamic modelling is required and calculation of emissions must be carried out using an appropriate method. Existing models use a range of empirical and theoretical formulae for calculation of emissions and, whilst empirical formulae may be appropriate in some cases, methods with a scientific basis should be used for all sources of emissions within the wastewater treatment plant in order to ensure that the effects of control strategies are reflected in the results.

Calculation of the energy requirement and associated indirect emissions could be improved by the use of a more detailed methodology, taking into account plant specific data, the design operating point of electrical equipment and relevant efficiency curves.

Dynamic modelling of N₂O emissions poses a particular challenge; emissions resulting from nitrification and denitrification in sludge treatment and nitrogen conversion in the digester effluent, for example, were only modelled by Préndez and Lara-González (2008) and the method utilised formulae based on activity

data and empirical emission factors. Keller and Hartley (2003) stated that N_2O emissions are not generally found in any significant quantity and are unlikely to contribute significantly to overall GHG emissions – however given that N_2O has a GWP 310 times greater than that of CO_2 (Defra 2011), even low emissions would have a considerable effect and Kampschreur et al. (2009) argued that N_2O emitted during wastewater treatment could significantly add to the carbon footprint. There have been recent investigations into the factors influencing N_2O emissions (Kampschreur et al. 2009, Foley et al. 2010, Rassamee et al. 2011), and it has been shown that N_2O generation is affected by process conditions such as DO concentration in the nitrification stage and COD/N ratio in the denitrification stage; however there is no consensus on a method which can be used to estimate emissions with any degree of certainty.

More detailed emission models for individual WWTP components exist, but would require incorporating into a model with wider scope to provide a comprehensive estimation of emissions. Ni et al. (2011), for example, developed a pseudo-mechanistic model to describe the production and consumption of N_2O during activated sludge nitrification and denitrification. This model has been tested using experimental data and, if combined with other models, could provide a flexible means of calculating N_2O emissions from the activated sludge unit. A potential disadvantage of combining detailed component models, however, is the increase in the overall model complexity and resultant increase in computational demand. To ensure suitability for multiple simulation runs and control strategy optimisation, it might be necessary to simplify the model following identification of the most important sources of GHG emissions using sensitivity analysis.

In conclusion, existing models for the assessment of GHG emissions from wastewater treatment differ vastly in both their choice of sources for inclusion and their estimation methodologies. None offer a comprehensive calculation of direct and indirect emissions and there are some potentially significant sources omitted from all. Challenges are posed by the need to calibrate models and to include emissions for which there are currently no reliable estimation methodologies.

It is thought that optimisation of control strategies could be used to reduce GHG emissions and contribute to carbon reduction requirements whilst maintaining

treatment standards. This would, however, require a model suitable for dynamic simulation, which is based upon theoretical relationships and would reflect the effects of changing operational conditions. Additional problems may be encountered when increasing the model detail and accuracy, due to the effect of increased computational demand on the simulation run time, particularly if optimisation is to be carried out.

2.2.8 Recent Developments

There have been some recent developments in the modelling of GHG emissions from wastewater treatment, including advances in the modelling of N₂O emissions and extensions to existing models. As these were published after completion of the model development stage of this research (and in some cases after submission of the thesis), they have not been included in this work in detail. However, a brief summary is provided below.

In particular, there have been significant advances in the modelling of N₂O emissions, with the development of extensions for existing activated sludge models. Guo and Vanrolleghem (2014), for example, have developed the activated sludge model for GHGs no. 1 (ASMG1). This includes an AOB denitrification model (Mampaey et al. 2013) to enable calculation of N₂O emissions resulting from the nitrification pathway, in addition to the N₂O emissions resulting from the denitrification pathway which have previously been modelled in ASMN (Hiatt and Grady 2008). Another model, ASMG2d (an extension of ASM2d), which includes phosphorus removal, has been developed by Guo (2014). A further addition in both ASMG1 and ASMG2d is the use of a modified Haldane kinetics term for description of the effect of DO on N₂O production by AOB.

The ASMG1 has also been incorporated in a later version of BSM2G (detailed by Flores-Alsina et al. (2014) and extended from the model discussed in Sections 2.2.1-2.2.6 (Flores-Alsina et al. 2011)). Further extensions here include modelling of emissions resulting from the stripping of dissolved gases from solutions, as by Foley et al. (2011).

The ASMG1 has been calibrated to fit N₂O emission data (Guo and Vanrolleghem 2014). However, the data used for calibration were from well-established models rather than real measurements, so the ability of the model

to reproduce measured data is unclear. Mechanistic models for production of N_2O by AOB, either by nitrifier denitrification or as a by-product of incomplete hydroxylamine oxidation, were compared and analysed by Ni et al. (2013). However, whilst these were generally found able to describe experimental ammonium, nitrate and nitrite data, none were able to consistently reproduce measured N_2O data and it was concluded that a unified model which captures potential interactions between the production mechanisms is required.

Following on from this, Ni et al. (2014) developed an integrated model which considers multiple N_2O production pathways by AOB. These include nitrifier denitrification (in which N_2O is the final product) and the hydroxylamine pathway (in which N_2O is emitted as a result of incomplete oxidation of NH_2OH to NO_2^-). Experimental data was used for calibration and validation of this model and it was found to provide satisfactory performance for two different systems. Ni et al. (2014) suggested that this model will enhance prediction of N_2O production by AOB under varying operational conditions.

Further extensions include development of a new mathematical model (ASM2d-SMP-GHG), which couples the ASM2d-SMP (Cosenza et al. 2013) and the ASMN (Hiatt and Grady 2008) for quantifying CO_2 and N_2O emissions in a membrane bioreactor (Mannina and Cosenza 2015). This does not include nitrifier denitrification, however, with the justification that models which include AOB denitrification are unable to reproduce measured data. It is also stated that a clear mathematical modelling approach has yet to be established for AOB denitrification (Mannina and Cosenza 2015), despite the recent developments. This corresponds with previous observation that different methods and models exist for describing N_2O production by AOB but there is conflict in their results, with some showing low DO concentrations maximise N_2O production whilst others suggest that high DO concentrations stimulate N_2O production (Guo et al. 2013, Ni et al. 2013).

Another method for quantification of N_2O emissions from full scale wastewater treatment systems with surface aerators, which integrates online monitoring, offline sampling, mathematical modelling and oxygen balance, has been presented by Ye et al. (2014). However, this has yet to be used in further study and validated. It is noted that empirical methods for analysis of N_2O emissions from wastewater treatment are also still being developed and used. Ali et al.

(2014), for example, presented empirical N_2O emission correlations for wastewater nitrification and suggested that these could be used to estimate and mitigate N_2O emissions from WWTPs.

In addition to models for N_2O production, there have also been developments in the modelling of CH_4 emissions. Daelman et al. (2014), for example, extended the ASM1 and BSM1 to investigate the fate of dissolved CH_4 in wastewater treatment and study the influence of process design and operational parameters on biological CH_4 oxidation. This involved modelling growth and decay of methanotrophs and modification of the aeration function to provide a more accurate description of the gas-liquid transfer of oxygen and CH_4 .

Despite these advances, however, there remain many challenges in the modelling and benchmarking of GHG emissions from wastewater treatment. Potential problems with a commonly used approach for modelling N_2O emissions from wastewater treatment – extending activated sludge models with process equations derived from batch experiments – have been noted by Snip et al. (2014): conditions for batch experiments are often different to those found in WWTPs and may not, therefore, be representative of full scale behaviour. When extending the ASM1 for modelling of N_2O formation during nitrification and denitrification (based on Hiatt and Grady (2008), Corominas et al. (2012) and Ni et al. (2013)), Snip et al. (2014) also identified problems related to the mathematical structure of the models. The need to check additional equations for inconsistencies, gaps, typing errors and coupling problems has consequently been emphasised (Snip et al. 2014). Further challenges are discussed by Vanrolleghem et al. (2014).

3 GREENHOUSE GAS EMISSIONS MODEL DEVELOPMENT

The WWTP emissions model developed within MATLAB/Simulink, which will be referred to as BSM2-e, incorporates the existing Benchmark Simulation Model No. 2 (BSM2) (Jeppsson et al. 2007) for dynamic biological process modelling and calculation of wastewater and sludge concentrations throughout the plant. GHG emissions are modelled using previously published estimation methodologies, which are implemented in the existing model. Modifications (outlined in Sections 3.2-3.3) are made to enable dynamic modelling of the emissions shown in Figure 3.1.

It must be noted that the results obtained from this model are not directly comparable with those from BSM2 due to alteration of the activated sludge model to include four-step denitrification.

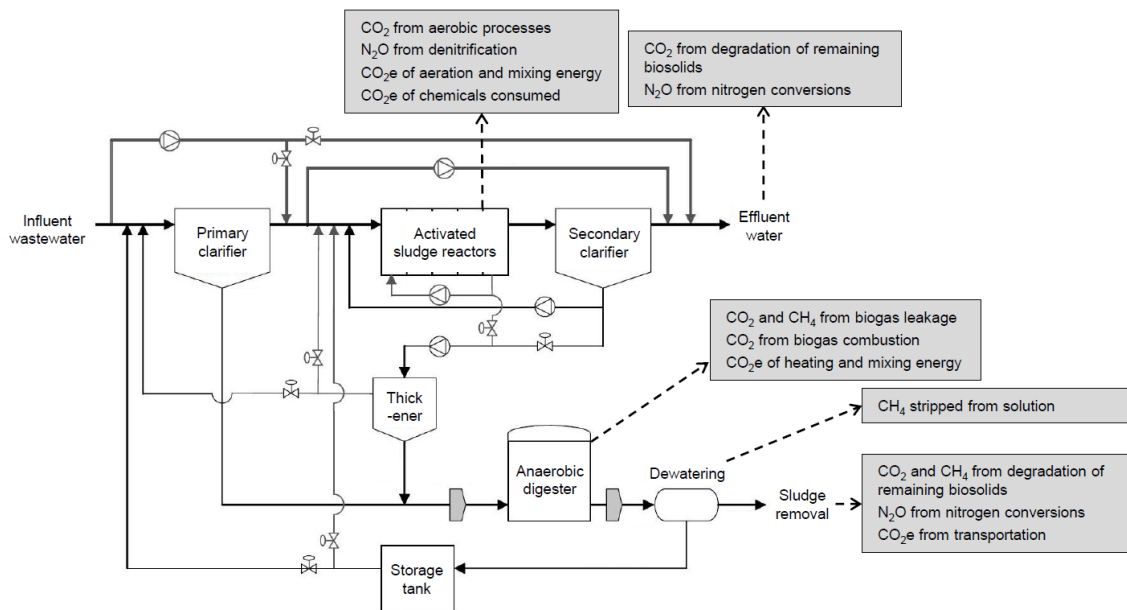


Figure 3.1: Schematic diagram of the modified BSM2 plant and sources of modelled GHG emissions (adapted from Nopens et al. 2010)

BSM2 enables calculation of indicators for performance assessment, based on a predefined plant layout and influent data and a user-defined control strategy. It was developed to enable the evaluation and comparison of control strategies, as this was previously difficult due to the use of different reference situations and a lack of standardised evaluation criteria (Alex et al. 2008). It is thought that the use of a recognised benchmark model within the GHG emissions model, for the evaluation of control strategies with respect to the effluent quality, will

enable greater flexibility when comparing the performance of newly developed and previously proposed control strategies.

3.1 Model Structure

The plant layout, shown in Figure 3.1, is unaltered from that of BSM2. The plant consists of a primary clarifier, an activated sludge unit containing five tanks in series, a secondary settler, a sludge thickener, an anaerobic digester, a dewatering unit and a storage tank. The activated sludge unit consists of an anoxic section, in which the nitrate level can be controlled by adjustment of the internal recycle flow rate, followed by three aerobic tanks in which the oxygen transfer coefficient can be controlled to change the DO level.

Adjustments (detailed in Section 3.2.1) have been made to the Activated Sludge Model No. 1 (ASM1) (Henze et al. 1987) used to describe biological phenomena in the reactors in BSM2, to enable calculation of N₂O emissions. Modelling of the remaining processes is as in BSM2 (detailed by Jeppsson et al. (2007) and Nopens et al. (2010)):

- The primary clarifier is modelled as a completely mixed tank with no biological reactions according to Otterpohl (1995), with a total suspended solids (TSS) removal efficiency of 50% and a HRT of 1 hour.
- The secondary clarifier is modelled based on Takács et al. (1991), assuming no biological activity.
- Thickening is modelled as an ideal, continuous process without biological reactions. A solids removal efficiency of 98% is assumed, with an underflow TSS concentration of 7%.
- Anaerobic digestion is modelled using ADM1 (Batstone et al. 2002), with a SRT of 19 days.
- The dewatering unit achieves a TSS concentration of 28%, providing 98% solids removal. The process is modelled as ideal and continuous and assumes no biological reactions occur.
- The storage tank is modelled as a continuous process with no biological activity.

3.2 Direct Emission Modelling Methodologies

3.2.1 Activated Sludge Reactors

Substrate Utilisation

Calculation of CO₂ emissions from substrate utilisation is based upon the method detailed by Monteith et al. (2005), with the suspended solids mass balance equation adapted for non-steady state conditions (i.e. $dX/dt \neq 0$), and it is assumed that CO₂ is formed during both substrate utilisation (biological oxidation) and biomass decay (auto-oxidation) in accordance with the stoichiometric equations presented (Eq. 2.5 and Eq. 2.7). Required concentrations and flow rates are derived from the BSM2 state variables and theoretical emission factors, derived from stoichiometry, are applied.

Each tank has only one inflow and one outflow (flow splitting and combining are modelled externally), so the suspended solids mass balance given by Monteith et al. (2005) is modified for application to each tank as follows to enable calculation of biomass formed in each reactor from substrate utilisation:

$$V \frac{dX}{dt} = Q_{in}X_{in} - Q_{out}X_{out} + VYr_s - Vk_dX \quad \text{Eq. 3.1}$$

where:

- V = reactor volume [m³]
- dX/dt = rate of change of biomass concentration in reactor [g VSS/m³/d]
- $Q_{in}X_{in}$ = biomass entering reactor in influent [g VSS/d]
- $Q_{out}X_{out}$ = biomass leaving reactor in effluent [g VSS/d]
- VYr_s = biomass formed in reactor from substrate utilisation [g VSS/d]
- Vk_dX = biomass decay in reactor [g VSS/d]

Of the five ASM1 state variables contributing to TSS, it is assumed that only active heterotrophic biomass ($X_{B,H}$) and active autotrophic biomass ($X_{B,A}$) can be classified as biomass. The rate of change of biomass concentration (dX/dt in Eq. 3.1) in each reactor at time i is, therefore, estimated using Eq. 3.2, based on the states modelled in BSM2. In data analysis, BSM2 uses time step durations calculated using the current simulation time and that at the following time step. To ensure model consistency, the rate of change of biomass concentration at each time step is therefore estimated based on output values at the current (t_i)

and subsequent (t_{i+1}) time steps, instead of using the previous time step or an alternative method.

$$\frac{dX}{dt} = \frac{\left(\frac{(X_{B,H} + X_{B,A})_{i+1}}{1.42} - \frac{(X_{B,H} + X_{B,A})_i}{1.42} \right)}{t_{i+1} - t_i} \quad \text{Eq. 3.2}$$

where:

$$1.42 = \text{conversion factor [g COD/g VSS]} \text{ (Comeau 2008)}$$

Biomass entering and leaving each reactor ($Q_{in}X_{in}$ and $Q_{out}X_{out}$ in Eq. 3.1) is calculated using Eq. 3.3:

$$\text{biomass mass flow rate [g VSS/d]} = Q \frac{X_{B,H} + X_{B,A}}{1.42} \quad \text{Eq. 3.3}$$

Biological processes modelled within ASM1 are based upon a cycle of biomass death and regeneration instead of growth and endogenous respiration, and therefore differ from the stoichiometric equations assumed to describe biomass decay and substrate utilisation for the purposes of emissions estimation. As such, some manipulation of the output data is therefore required to enable application of Eq. 3.1, and the rate of biomass decay (Vk_dX in Eq. 3.1) is calculated using the biomass concentration derived from the BSM2 outputs and the reactor volume, as shown in Eq. 3.4:

$$\text{rate of biomass decay [g VSS/d]} = V k_{d,T} \frac{X_{B,H} + X_{B,A}}{1.42} \quad \text{Eq. 3.4}$$

where:

$$k_{d,T} = \text{endogenous decay coefficient at temperature } T$$

Temperature dependency of k_d is modelled as for the heterotrophic decay coefficient in BSM2, using a base value of 0.3 d^{-1} (b_H , defined in BSM2) and the current activated sludge temperature (T_{as}) output from the model:

$$k_{d,T} = b_H \exp \left(\left(\frac{\ln \left(\frac{b_H}{0.2} \right)}{5} \right) (T_{as} - 15) \right) \quad \text{Eq. 3.5}$$

The rate of biomass formation in each reactor (VYr_s) is then derived from Eq. 3.1. The heterotrophic cell yield coefficient, Y , defined in BSM2 (0.67 g VSS/g COD) is used to calculate the aeration BOD₅ removal rate (r_s) and the oxygen removal rate due to the oxidation of substrate is then calculated using Eq. 3.6 (Monteith et al. 2005). A theoretical emission factor of 1.1 g CO₂/g O₂ (EF_{AerOxi}) (Monteith et al. 2005), derived from stoichiometry (Eq. 2.5), is applied to calculate CO₂ production from aerobic oxidation:

$$r_{O_2} = \frac{Vr_s}{f} - 1.42Vr_sY \quad \text{Eq. 3.6}$$

$$CO_{2,AS,BOD} = \sum_{i=1}^5 EF_{AerOxi} \times r_{O_2,i} \quad \text{Eq. 3.7}$$

where:

- r_{O_2} = oxygen removal rate due to substrate oxidation [g O₂/ d]
- Vr_s/f = total rate of BOD_u removal in reactor (due to both substrate oxidation and biosynthesis) [g BOD_u/d]
- $1.42Vr_sY$ = BOD_u removal due to biosynthesis (in which no CO₂ is formed) [g COD/d]
- f = conversion factor, set to 0.68 g BOD₅/g BOD_u (Monteith et al. 2005)
- Y = cell yield coefficient [g VSS/g COD]
- i = tank number

Biomass Decay

Calculation of CO₂ from biomass decay is also based upon the method detailed by Monteith et al. (2005), with required concentrations and flow rates derived from BSM2.

The rate of CO₂ production due to biomass decay is modelled for each reactor using a theoretical emission factor of 1.947 kg CO₂/kg VSS ($EF_{AerAutoOxi}$) (Monteith et al. 2005). The total rate of CO₂ production (g CO₂/d) due to biomass decay in the activated sludge process is therefore calculated using Eq. 3.8.

$$CO2_{AS,VSS} = \sum_{i=1}^5 EF_{AerAutoOxi} \times (Vk_{d,TX})_i \quad \text{Eq. 3.8}$$

Denitrification

In BSM2, the reduction of nitrate to nitrogen is modelled as a one-step process and dynamic production of N₂O (an intermediate product) cannot be determined. The activated sludge model has, therefore, been modified to include four-step denitrification as detailed by Samie et al. (2011) (based on the ASMN developed by Hiatt and Grady (2008)), to enable dynamic modelling of CO₂ and N₂O production during denitrification.

All processes and process rates in the model are detailed in Table 3.1 and reactions are detailed in Table 3.2. Processes A-D replace the single step in BSM2 for anoxic growth of heterotrophs and the single variable used in BSM2 for 'nitrate and nitrite nitrogen' (S_{NO}) is replaced with separate variables for nitrate (S_{NO3}), nitrite (S_{NO2}), nitric oxide (S_{NO}) and nitrous oxide nitrogen (S_{NO}).

Note that the model detailed by Samie et al. (2011) is not a complete implementation of the ASMN. Given that the aim of the study was to model N₂O emissions and only enhancements to modelling of the denitrification process in ASMN provide additional functionality in this respect, only modelling of the denitrification process was modified by Samie et al. (2011), with the single step denitrification of ASM1 replaced with four-step denitrification as described by Hiatt and Grady (2008). Modelling of nitrification remains as in ASM1 (i.e. a single process without inhibition) instead of using two autotrophic processes (ammonia oxidation and nitrite oxidation) as in ASMN, and assimilative nitrite reduction to ammonia and biodegradation of specific organic components are not added.

Samie et al. (2011) found the model with a partial implementation of ASMN to provide a very good fit with measured values, suggesting that it performs sufficiently well for use in further study. However, it is recognised that the simple modelling of nitrification and lack of inhibition modelling will affect results under elevated nitrogen conditions and inhibition.

Table 3.1: Modified ASM1 process rates, adapted from Samie et al. (2011) and Alex et al. (2008)

Process	Process rate
1 Aerobic growth of heterotrophs	$\mu_{HT} \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{S_O}{K_{O,H} + S_O} \right) X_{B,H}$
A Anoxic growth of heterotrophs on nitrate	$\mu_{HT} \left(\frac{S_S}{K_{S2} + S_S} \right) \left(\frac{K_{O,H2}}{K_{O,H2} + S_O} \right) \left(\frac{S_{NO3}}{K_{NO3} + S_{NO3}} \right) \eta_{g2} X_{B,H}$
B Anoxic growth of heterotrophs on nitrite	$\mu_{HT} \left(\frac{S_S}{K_{S3} + S_S} \right) \left(\frac{K_{O,H3}}{K_{O,H3} + S_O} \right) \left(\frac{S_{NO2}}{K_{NO2} + S_{NO2}} \right) \left(\frac{K_{13NO}}{K_{13NO} + S_{NO}} \right) \eta_{g3} X_{B,H}$
C Anoxic growth of heterotrophs on nitric oxide	$\mu_{HT} \left(\frac{S_S}{K_{S4} + S_S} \right) \left(\frac{K_{O,H4}}{K_{O,H4} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO} + \frac{S_{NO}^2}{K_{14NO}}} \right) \eta_{g4} X_{B,H}$
D Anoxic growth of heterotrophs on nitrous oxide	$\mu_{HT} \left(\frac{S_S}{K_{S5} + S_S} \right) \left(\frac{K_{O,H5}}{K_{O,H5} + S_O} \right) \left(\frac{S_{N2O}}{K_{N2O} + S_{N2O}} \right) \left(\frac{K_{15NO}}{K_{15NO} + S_{NO}} \right) \eta_{g5} X_{B,H}$
3 Aerobic growth of autotrophs	$\mu_{AT} \left(\frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left(\frac{S_O}{K_{O,A} + S_O} \right) X_{B,A}$
4 Decay of heterotrophs	$b_{HT} X_{B,H}$
5 Decay of autotrophs	$b_{HT} X_{B,A}$
6 Ammonification of soluble organic nitrogen	$k_{aT} S_{ND} X_{B,H}$
7 Hydrolysis of entrapped organics	$k_{hT} \frac{X_S/X_{B,H}}{K_X + (X_S/X_{B,H})} \left(\left(\frac{S_O}{K_{O,H} + S_O} \right) + \eta_h \left(\frac{K_{O,H}}{K_{O,H} + S_O} \right) \left(\frac{S_{NO3} + S_{NO2}}{K_{NO} + S_{NO3} + S_{NO2}} \right) \right) X_{B,H}$
9 Hydrolysis of entrapped organic nitrogen	$k_{hT} \frac{X_S/X_{B,H}}{K_X + (X_S/X_{B,H})} \left(\left(\frac{S_O}{K_{O,H} + S_O} \right) + \eta_h \left(\frac{K_{O,H}}{K_{O,H} + S_O} \right) \left(\frac{S_{NO3} + S_{NO2}}{K_{NO} + S_{NO3} + S_{NO2}} \right) \right) X_{B,H} \left(\frac{X_{ND}}{X_S} \right)$
10 Stripping of N ₂ O to atmosphere	$kLa_{N2O} (S_{N2Os} - 28K_{H,N2O} P_{N2O})$

Table 3.2: Modified ASM1 stoichiometry matrix, adapted from Samie et al. (2011) and Alex et al. (Alex et al. 2008)

Process	Model component																
	S _I	S _S	X _I	X _S	X _{B,H}	X _{B,A}	X _P	S _{O2}	S _{NO3}	S _{NH}	S _{ND}	X _{ND}	S _{ALK}	S _{NO2}	S _{NO}	S _{N2O}	
1		$-\frac{1}{Y_H}$			+1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$				
A		$-\frac{1}{Y_H\eta_Y}$			+1			$-\frac{1-Y_H\eta_Y}{1.143Y_H\eta_Y}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$+\frac{1-Y_H\eta_Y}{1.143Y_H\eta_Y}$			
B		$-\frac{1}{Y_H\eta_Y}$			+1					$-i_{XB}$			$+\frac{1-Y_H\eta_Y}{14\times 0.571Y_H\eta_Y}$ $-\frac{i_{XB}}{14}$	$-\frac{1-Y_H\eta_Y}{0.571Y_H\eta_Y}$	$+\frac{1-Y_H\eta_Y}{0.571Y_H\eta_Y}$		
C		$-\frac{1}{Y_H\eta_Y}$			+1					$-i_{XB}$			$-\frac{i_{XB}}{14}$		$-\frac{1-Y_H\eta_Y}{0.571Y_H\eta_Y}$	$+\frac{1-Y_H\eta_Y}{0.571Y_H\eta_Y}$	
D		$-\frac{1}{Y_H\eta_Y}$			+1					$-i_{XB}$			$-\frac{i_{XB}}{14}$			$-\frac{1-Y_H\eta_Y}{0.571Y_H\eta_Y}$	
3						+1		$-\frac{4.57-Y_A}{Y_A}$	$+\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$				
4				$+1-f_P$	-1		$+f_P$					$+i_{XB}$ $-f_Pi_{XP}$					
5				$+1-f_P$		-1	$+f_P$					$+i_{XB}$ $-f_Pi_{XP}$					
6										+1	-1		$+\frac{1}{14}$				
7		+1		-1													
8											+1	-1					
9																-1	
Units	COD							- COD	N				Mole	N			

In addition to the reactions modelled by Samie et al. (2011), allowance is made for the stripping N₂O from solution, which results in emission to the atmosphere. The rate of N₂O emission from each reactor is dependent on temperature and dissolved N₂O concentration, and is modelled using Eq. 3.9. Temperature dependency of the Henry's law constant is modelled in accordance with the ADM1 methodology for CO₂ and CH₄ stripping, using a base value of 0.025 mol/l/atm at 298.15 K (Lide and Frederiske, 1995; quoted in NIST 2012).

$$r_{N2Og} = 3.14kLa_{N2O} \times \max\left(0, (S_{N2Os} - 28 \times 1000K_{H,N2O}Pgas_{N2O})\right) \quad \text{Eq. 3.9}$$

where:

- r_{N2Og} = rate of N₂O emissions [g N₂O/m³/d]
- 3.14 = conversion factor from g N to g N₂O [g N₂O/g N]
- kLa_{N2O} = N₂O gas transfer coefficient, set to 2 d⁻¹ (Samie et al. 2011)
- 28 = conversion factor [g N/mol N₂O]
- 1000 = conversion factor [l/m³]
- $K_{H,N2O}$ = Henry's law constant for N₂O [mol N₂O/kg/atm]
- $Pgas_{N2O}$ = partial pressure of N₂O in atmosphere, set to 3.2 × 10⁻⁷ atm (European Environment Agency 2011)

The total rate of N₂O emission from the five activated sludge tanks at each time step is therefore calculated using Eq. 3.10.

$$N2O_{AS,deni} = \sum_{i=1}^5 r_{N2Og,i} V_i \quad \text{Eq. 3.10}$$

CO₂ emissions resulting from nutrient removal are calculated using the stoichiometric relationships given by Shahabadi et al. (2010) for denitrification with and without an external carbon source (Eq. 2.12 and Eq. 2.13)

Given that these stoichiometric relationships are for complete denitrification and some nitrate removed in the model may be only partially denitrified, emission factors are derived to enable calculation of CO₂ emissions from denitrification based on the mass of nitrogen (N₂) produced instead of the mass of nitrate removed. This yields factors of 2.62 g CO₂/g N₂-N ($EF_{CO2denitWCarb}$) and 2.83 g CO₂/g N₂-N ($EF_{CO2denitWOCarb}$) for denitrification with and without an

external source respectively. Production of N_2 at each time step is modelled as follows:

$$r_{N_2} = \left(\frac{1 - Y_H \eta_Y}{0.571 Y_H \eta_Y} \right) procD \quad \text{Eq. 3.11}$$

where:

- r_{N_2} = rate of N_2 production [g N/m³/d]
- Y_H = heterotrophic biomass yield [g COD/g COD]
- η_Y = anoxic yield factor for heterotrophs
- $procD$ = process rate D, defined in Table 3.1

It is assumed that the emission factor for denitrification with an external carbon source is valid even for very low carbon source flow rates (Q_{carb}), provided that $Q_{carb} > 0$. The total rate of CO_2 emissions resulting from denitrification in the activated sludge is given by Eq. 3.12:

$$CO2_{AS,deni} = \sum_{i=1}^5 E_i r_{N_2,i} V_i \quad \text{Eq. 3.12}$$

where:

- E_i = CO_2 emission factor ($EF_{CO2denitWCarb}$ when $Q_{carb} > 0$, else $EF_{CO2denitWOCarb}$)

Total Activated Sludge Reactor Emissions

The total rate of GHG emissions from the reactor at each time step ($CO2e_{AS,total}$) is modelled using Eq. 3.13.

$$CO2e_{AS,total} = CO2_{AS,VSS} + CO2_{AS,BOD} + CO2_{AS,deni} + 310 \times N2O_{AS,deni} \quad \text{Eq. 3.13}$$

3.2.2 Biogas Leakage and Combustion

Dynamic CH_4 and CO_2 formation and stripping in the anaerobic digester and the resultant biogas composition and flow rate are modelled using the BSM2 methodology. Dissolved CH_4 is not accounted for prior to the ASM to ADM interface, and is therefore assumed to be zero on entry to the digester. Total production of gaseous CH_4 and CO_2 in the anaerobic digester is calculated using Eq. 3.14 and Eq. 3.15 respectively:

$$CH4_{AD,biogas} = \frac{p_{gas,ch4}}{P_{gas,total}} Q_{gas} P_{atm} \frac{16}{RT} \quad \text{Eq. 3.14}$$

$$CO2_{AD,biogas} = \frac{p_{gas,co2}}{P_{gas,total}} Q_{gas} P_{atm} \frac{44}{RT} \quad \text{Eq. 3.15}$$

where:

$CH4_{AD,biogas}$ = total CH₄ content of biogas [kg CH₄/d]

$CO2_{AD,biogas}$ = total CO₂ content of biogas [kg CO₂/d]

$p_{gas,i}$ = partial pressure of gas i

$P_{gas,total}$ = digester gas pressure [bar]

Q_{gas} = gas flow rate [m³/d]

P_{atm} = atmospheric pressure [bar]

16 = conversion factor [g CH₄/mol CH₄]

44 = conversion factor [g CO₂/mol CO₂]

R = molar gas constant [bar m³/K/kmol]

T = digester temperature [K]

It is assumed in BSM2 that all biogas (except that which remains in solution) is combusted for energy recovery. However, past investigations (e.g. Shahabadi et al. 2009, Shahabadi et al. 2010), have identified biogas leakage as a potential contributor to total emissions. As it is impractical to accurately measure or model small leaks, a fixed leakage factor of 5% (Georges et al. 2009, Shahabadi et al. 2009) has been applied. Leaked gas includes both CH₄ and CO₂ in the same proportions as in the digester biogas. It is assumed that the remaining biogas is fully combusted in accordance with Eq. 2.14, which yields an emission factor of 2.75 g CO₂/g CH₄ (Monteith et al. 2005).

Total emissions of CH₄ ($CH4_{AD}$) and CO₂ ($CO2_{AD}$) to the atmosphere from the anaerobic digester are, therefore, calculated using Eq. 3.16 and Eq. 3.17 respectively.

$$CH4_{AD} = 0.05 \times CH4_{AD,biogas} \quad \text{Eq. 3.16}$$

$$CO2_{AD} = CO2_{AD,biogas} + 2.75 \times 0.95 \times CH4_{AD,biogas} \quad \text{Eq. 3.17}$$

The rate of total direct emissions from the anaerobic digester ($CO2e_{AD,total}$) at each time step is calculated as follows:

$$CO2e_{AD,total} = CO2_{AD} + 21 \times CH4_{AD} \quad \text{Eq. 3.18}$$

3.2.3 Stripping of Dissolved Gases in Dewatering Unit

The concentration of CH_4 dissolved in the digester effluent is calculated in BSM2, based on a mass balance including the gas transfer rate and CH_4 formation during the uptake of acetate and hydrogen. However, as BSM2 is only interested in CH_4 production in respect to the energy that can be recovered, progression of this dissolved CH_4 through the plant is not modelled and data is lost at the ADM to ASM interface (where the variables used to define the current states are altered). In the modified emissions model, it is assumed that this CH_4 remains in solution as the sludge progresses to the dewatering unit and that the concentration of dissolved CH_4 in sludge entering the dewatering unit is equal to that in sludge leaving the anaerobic digester at the corresponding time step.

Given that the partial pressure of CH_4 in the atmosphere is negligible, it is expected that no CH_4 would remain in solution. The CH_4 mass flow rate ($CH4_{dewatering}$) from the dewatering unit at each time step is therefore modelled using Eq. 3.12. This is converted into units of CO_2e using Eq. 3.20.

$$CH4_{dewatering} = \frac{16}{64} \times S_{ch4} Q \quad \text{Eq. 3.19}$$

$$CO2e_{dewatering} = 21 \times CH4_{dewatering} \quad \text{Eq. 3.20}$$

where:

- 16 = conversion factor [g CH_4 /mol CH_4]
- 64 = conversion factor [g COD/mol CH_4]
- S_{ch4} = dissolved CH_4 concentration [g COD/m³]
- Q = sludge flow rate [m³/d]

The gas transfer rate (assumed to be 200 d⁻¹ for CH_4 in the digester in BSM2) is not taken into account for stripping of CH_4 from solution in the dewatering unit as it is assumed that all dissolved CH_4 will be stripped eventually, and it would therefore have no effect on net emissions. Its absence will affect the rate of

emissions modelled and might result in offsite emissions being attributed to the dewatering unit if stripping is slow; however, since CH₄ is not included after the ADM to ASM interface, this approach prevents CH₄ becoming ‘lost’ in the modelling system and remaining unaccounted for.

3.3 Indirect Emission Modelling Methodologies

3.3.1 Generation of Energy Imported

Pumping Energy Requirements

Energy required for pumping at each time step is calculated using the BSM2 methodology. Pumps are modelled at six locations in the system, as detailed in Table 3.3. Influent pumping is not modelled in BSM2 given that this is not affected by the WWTP control and its inclusion is not necessary for comparison of operational costs under different control strategies. The same approach is applied for GHG emissions. It is assumed that the energy consumption of each pump is linearly related to the volume of water pumped and different energy factors are used at each location, as summarised in Table 3.3.

Table 3.3: Pumping energy factors used in BSM2 (Alex et al. 2008)

Pump location	Energy factor [kWh/m ³]
Internal activated sludge recirculation	0.004
Activated sludge recycle	0.008
Activated sludge wastage flow	0.05
Primary clarifier underflow	0.075
Thickener underflow	0.06
Dewatering underflow	0.008

The total rate of energy consumption for pumping at each time step ($E_{pumping}$) is calculated using the modelled flow rates at each pump location, Q_j , and corresponding energy factors, F_j :

$$E_{pumping} = \sum_j Q_j F_j \quad \text{Eq. 3.21}$$

Use of the BSM2 method to model pumping energy does not take into account variations in efficiency; if pumps are not operating at their design capacity, the energy consumption may be significantly higher than calculated. However pumping energy contributes to the BSM2 operational cost index in performance

assessment and therefore should not be altered if comparisons are to be drawn with previously developed control strategies. If the emissions model is adapted for application to a case study WWTP, then it may be beneficial to incorporate site-specific information regarding pump efficiency and operating curves.

Aeration Energy Requirements

Energy required for aeration of the activated sludge reactors is calculated using the BSM2 methodology, which is valid for Degremont DP230 porous disks at an immersion depth of 4 m (Alex et al. 2008). The energy consumption at each time step is dependent on the corresponding oxygen transfer coefficients, which can be altered throughout the simulation duration to control the aeration intensity in each tank. The total rate of energy consumption for aeration at each time step ($E_{aeration}$) is calculated using Eq. 3.22 (adapted from Alex et al. 2008):

$$E_{aeration} = \sum_{i=1}^5 \frac{S_O^{sat}}{1.8 \times 1000} V_i (K_L a)_i \quad \text{Eq. 3.22}$$

where:

- S_O^{sat} = oxygen saturation concentration = 8 mg O₂/l
- 1.8 = aeration oxygen transfer efficiency [mg O₂/kWh]
- 1000 = unit conversion factor [l/m³]
- V = tank volume [m³]
- $K_L a$ = oxygen transfer coefficient [d⁻¹]

This method assumes a linear relationship between aeration energy and O₂ supplied, making no allowance for variations in efficiency. Furthermore, temperature dependence of the oxygen saturation concentration is not modelled, despite it being included in the BSM2 activated sludge model. However, as for the pumping energy, aeration energy calculated using this method contributes to the BSM2 operational cost index and modification would affect the suitability of the emissions model for assessment of previously proposed control strategies. A more detailed method could be applied on a site-specific basis.

Heating Energy Requirements

The energy required theoretically to heat the anaerobic digester is modelled in BSM2, based on the sludge specific heat capacity. The digester receives inflows from the primary clarifier ($Q_{AD,clar}$) and the thickener ($Q_{AD,thick}$) and a weighted average of the influent temperatures ($T_{AD,clar}$ and $T_{AD,thick}$) is used to calculate the rate of energy consumption ($E_{heating}$) required to raise the temperature to 35°C at each time step (adapted from Alex et al. 2008):

$$T_{AD,in} = \frac{Q_{AD,clar}T_{AD,clar} + Q_{AD,thick}T_{AD,thick}}{Q_{AD,clar} + Q_{AD,thick}} \quad \text{Eq. 3.23}$$

$$E_{heating} = \frac{24(35 - T_{AD,in})Q \rho c}{86400} \quad \text{Eq. 3.24}$$

where:

- 24 = conversion factor [h/d]
- ρ = sludge density [kg/m^3]
- c = sludge specific heat capacity [$\text{W s/g}^\circ\text{C}$]
- 86400 = conversion factor [s/d]

In BSM2, it is assumed that the sludge can be characterised using the density and specific heat capacity of water: 1000 kg/m^3 and $4.186 \text{ W s/g}^\circ\text{C}$ respectively.

Mixing Energy Requirements

Energy required for mixing the activated sludge reactors and the anaerobic digester is modelled in BSM2. The activated sludge reactors are only mixed when the corresponding oxygen transfer coefficient is less than 20 d^{-1} but the digester is mixed constantly. The rates of energy consumption at each time step for mixing the five activated sludge tanks ($E_{mixingAS}$) and the digester ($E_{mixingAD}$) are calculated using Eq. 3.25 and Eq. 3.26 respectively:

$$E_{mixingAS} = \sum_{i=1}^5 0.005 \times 24 V_i \text{ if } (K_L a)_i < 20 \text{ d}^{-1} \quad \text{Eq. 3.25}$$

else 0

$$E_{mixingAD} = 0.005 \times 24 V_{liq} \quad \text{Eq. 3.26}$$

where:

$$\begin{aligned}
0.005 &= \text{mixing energy factor [kW/m}^3\text{]} \\
24 &= \text{conversion factor [h/d]} \\
V_{liq} &= \text{anaerobic digester liquid volume [m}^3\text{]}
\end{aligned}$$

Use of this method implies that activated sludge mixing energy is dependent only the tank volume and involves the assumption that it is not affected by factors such as flow rate. No provision is made for different mixing intensities: it is simply on or off.

Biogas Energy Recovery

It is assumed that biogas is combusted for heating of the anaerobic digester; electricity generation is considered not to occur. Energy recovery from biogas combustion is calculated based on the modelled rate of CH₄ production (Eq. 3.14), but reduced by 5% with respect to the BSM2 value to account for the 5% biogas leakage. The rate of energy recovery at each time step (E_{credit}) is calculated with Eq. 3.27, using the theoretical energy content of CH₄ and a conversion efficiency factor of 0.50 (Gori et al. 2011).

$$E_{credit} = 0.95 \times CH4_{AD,biogas} \times \frac{50014}{3600} \times CF \quad \text{Eq. 3.27}$$

where:

$$\begin{aligned}
50014 &= \text{theoretical CH}_4 \text{ energy content [J/kg]} \\
3600 &= \text{conversion factor [J/kWh]} \\
CF &= \text{energy conversion efficiency}
\end{aligned}$$

Net Energy Import and Associated Emissions

The net rate of energy import at each time step is dependent on the total plant energy consumption and the energy recovery from biogas combustion. The original BSM2 methodology assumes that energy recovered from biogas can be used to offset energy imported at any stage in the evaluation period; however this assumption is only valid if any excess energy is stored, as no checks are made to ensure that there is sufficient onsite demand to immediately use all energy as it is generated. Given that the energy generated may not be enough to justify installation of a system to store excess or return it to the grid, the rate of net energy import for heating ($E_{heating,net}$) and electricity ($E_{electricity,net}$) is

modelled at each time step, using Eq. 3.28 and Eq. 3.29 if recovered energy is used for heating or Eq. 3.30 and Eq. 3.31 if used for electricity generation.

$$E_{heating,net} = \max(0, E_{heating} - E_{credit}) \quad \text{Eq. 3.28}$$

$$E_{electricity,net} = E_{pumping} + E_{aeration} + E_{mixingAS} + E_{mixingAD} \quad \text{Eq. 3.29}$$

$$E_{heating,net} = E_{heating} \quad \text{Eq. 3.30}$$

$$E_{electricity,net} = \max(0, E_{pumping} + E_{aeration} + E_{mixingAS} + E_{mixingAD} - E_{credit}) \quad \text{Eq. 3.31}$$

The rate of indirect emissions at each time step due to net energy import (CO_2e_{energy}) is modelled using Eq. 3.32.

$$CO_2e_{energy} = 0.245(E_{heating,net} + E_{electricity,net}) \quad \text{Eq. 3.32}$$

GHG emissions associated with net energy import are affected by the electricity generation mix, as emissions differ between energy sources. However, as electricity grid composition varies locally and nationally and the model is not linked to a specific location, a single emission factor of 0.245 kg CO₂e/kWh (Gori et al. 2011) is used.¹

¹ ADDENDUM: In the model development, a range of emission factors reported in literature were evaluated. A value of 0.245 kg CO₂e/kWh (Gori et al. 2011) was ultimately selected as it yielded GHG emissions resulting from net electricity import most similar to those reported by Flores-Alsina et al. (2011) for the same model under the same control strategy (despite a higher emission factor being used in their model). It has since been ascertained that this is due to differences in the modelling of energy recovery: electricity generation is not included in BSM2-e, hence the net electricity import is higher and a lower emission factor is required to give the same level of emissions.

Emission factors differ between countries, and even within countries and from year to year, due to changes in the fuel mix consumed in power stations and the contribution of renewables. Indeed, the chosen emission factor is not unrealistic since values in the range of 0.000 to 1.787 kg CO₂e/kWh have been reported by the International Energy Agency (2013). Several European countries have a reported emission factor of less than 0.245 kg CO₂e/kWh, including Norway, Sweden, Switzerland, France, Finland, Belgium and Austria (International Energy Agency 2013). However, in retrospect, a higher emission factor of 0.484 kg CO₂e/kWh, in line with that provided by Defra (2013) for electricity consumed from the UK national grid, may have been more appropriate for use in this study.

Use of an emission factor of 0.484 kg CO₂e/kWh in BSM2-e would increase indirect emissions resulting from energy use by 97.6%: however, this would only increase total emissions from the plant by 5.7% in the default open loop scenario, and by 4.9% under the default closed loop control strategy. Clearly any model changes would be expected to have some impact on the results of sensitivity analysis (Chapters 4 and 5) and control strategy optimisation (Chapter 6), even if only small, and it is recommended that future application of the methodologies demonstrated in this thesis to a real WWTP utilise an emission factor selected on a case-specific basis.

3.3.2 Manufacture of Chemicals

Indirect emissions due to chemical addition have been calculated using the carbon source flow rate for each tank, as modelled in BSM2, and an emission factor of 1.54 kg CO₂e/kg MeOH (Shahabadi et al. 2010). It is specified in BSM2 that the carbon source has a concentration of 400 kg COD/m³ and, given that methanol has a theoretical oxygen demand of 1.5 g COD/g MeOH, the rate of associated emissions is calculated using Eq. 3.33:

$$CO2e_{methanol} = \sum_{i=1}^5 \frac{Q_{C,i} \times 400}{1.5} \times 1.54 \quad \text{Eq. 3.33}$$

where:

$$Q_C = \text{carbon source flow rate [m}^3\text{/d]}$$

Further additives may include polymers and coagulants, for example. However, as these are not included in BSM2, they cannot be adjusted in the control options evaluated and their associated emissions would not change. They are not, therefore, considered in this work.

3.3.3 Offsite Degradation of Effluent

Indirect CO₂ emissions from the reactor effluent are modelled using Eq. 3.34, based on the assumption that all BOD₅ remaining in the effluent degrades aerobically in accordance with the stoichiometric equation given by Shahabadi et al. (2010), which yields an emission factor of 0.33 g CO₂/g BOD ($EF_{AerBODrem}$). Effluent BOD (BOD_{eff}) is calculated using the BSM2 methodology.

$$CO2_{eff} = BOD_{eff} \times EF_{AerBODrem} \quad \text{Eq. 3.34}$$

The rate of indirect N₂O emissions from the reactor effluent are calculated using the total effluent nitrogen concentration (N_{eff}) modelled in BSM2 and an emission factor of 0.005 kg N₂O-N/kg N (IPCC 2006b), as shown in Eq. 3.35.

$$N2O_{eff} = 0.005 \times \frac{44}{28} \times N_{eff}Q \quad \text{Eq. 3.35}$$

where:

$$44/28 = \text{conversion factor [g N}_2\text{O/g N}_2\text{O-N]}$$

The total rate of GHG emissions from the reactor time step is calculated using Eq. 3.36:

$$CO2e_{effluent} = CO2_{effluent} + 310 \times N2O_{effluent} \quad \text{Eq. 3.36}$$

3.3.4 Transport and Offsite Degradation of Sludge

Dynamic simulation of emissions resulting from sludge disposal is based on digester effluent concentrations and flow rates modelled in BSM2. Calculation of the mass of sludge for disposal over the one-year evaluation period in BSM2 also includes net accumulation of sludge in the primary clarifier, activated sludge reactors, each layer of the secondary clarifier and the storage tank over the simulation period. However, TSS concentrations in these units are subject to large fluctuations, so it would be unreasonable to include sludge accumulation in the WWTP when modelling the rate of sludge production for disposal at each time step. Dynamic simulation of emissions resulting from sludge disposal is therefore based on only the digester effluent following dewatering, with accumulation in the WWTP excluded.

Emissions resulting from the transport of sludge produced for disposal at each time step are estimated using Eq. 3.37, with an emission factor ($EF_{sludge,trans}$) of 24 kg CO₂e/tonne solids (Shahabadi et al. 2010).

$$CO2e_{sludge,trans} = EF_{sludge,trans} \times TSS \times Q \quad \text{Eq. 3.37}$$

Indirect emissions resulting from the degradation of biosolids remaining in the sludge are modelled using the method detailed by Shahabadi et al. (2009), based on the theoretical stoichiometric equation for biomass decay in an anaerobic environment (Eq. 2.4). It is assumed that the degradable suspended solids in the sludge can be represented by the readily biodegradable substrate (S_s) modelled in BSM2; the rates of CO₂ and CH₄ emissions resulting from the degradation of sludge produced at each time step are, therefore, calculated using Eq. 3.38 and Eq. 3.39 respectively.

$$CO2_{sludge} = EF_{AnaerVSSdecCO2} \times \frac{S_s}{1.42} Q \quad \text{Eq. 3.38}$$

$$CH4_{sludge} = EF_{AnaerVSSdecCH4} \times \frac{S_s}{1.42} Q \quad \text{Eq. 3.39}$$

where:

$EF_{AnaerVSSdecCO_2}$ = theoretical CO_2 emission factor, set to 0.58 g CO_2 /g VSS
(Shahabadi et al. 2010)

$EF_{AnaerVSSdecCH_4}$ = theoretical CH_4 emission factor, set to 0.35 g CH_4 /g VSS
(Shahabadi et al. 2010)

N_2O emissions resulting from sludge produced for disposal at each time step are calculated using the total nitrogen content modelled in BSM2 and an emission factor ($EF_{sludgeN_2O}$) of 0.01 kg N_2O -/kg N, as recommended by the IPCC (2006a) for application of sludge to managed soils:

$$N_2O_{sludge} = EF_{sludge,N_2O} \times \frac{44}{28} \times N_{effluent,total} Q \quad \text{Eq. 3.40}$$

The overall rate of emissions resulting from the disposal of sludge at each time step is therefore calculated using Eq. 3.41.

$$CO_2e_{sludge} = CO_2e_{sludge,trans} + CO_2e_{sludge} + 21 \times CH_4_{sludge} + 310 \times N_2O_{sludge} \quad \text{Eq. 3.41}$$

3.4 Emission Source Omissions

Additional direct emissions may result from poorly managed treatment and unintentionally anaerobic conditions (Monteith et al. 2005); these are not modelled, however, due to a lack of reliable estimation techniques. Likewise, N_2O emissions associated with nitrifier denitrification during nitrification are also omitted due to a lack of suitable modelling techniques – metabolic models exist (Ni et al. 2011, Mampaey et al. 2013) but have been found unable to accurately and consistently reproduce experimental data (Law et al. 2012a, Ni et al. 2013, Sperandio et al. 2014).

The significance of these omissions is uncertain, as previous field studies have identified CH_4 emissions from every processing unit (Wang et al. 2011) and nitrifier denitrification is known to yield high N_2O emissions relative to the mass of nitrogen converted, although the proportion of nitrogen removal attributed to this pathway is hard to determine (Kampschreur et al. 2009). Incomplete hydroxylamine oxidation can also result in N_2O emissions, but it is unclear under what conditions this process becomes dominant and current models are

inadequate (Ni et al. 2013). If these sources are included in future GHG emission estimates for control strategy development, further work to investigate their variance resulting from the choice of control handle values is recommended.

3.5 Simulation Strategy

Under the BSM2 simulation strategy, performance is assessed using a 609 day dynamic simulation with predefined dynamic influent data. The first 245 days are used to achieve pseudo steady state and allow controllers to adapt and the final 364 days are used for performance evaluation, with model states output at 15 minute intervals. The dynamic simulation should be preceded by 200 days of constant influent (representing average values from the dynamic data), from which the steady state values obtained are used as initial values for dynamic simulation (Jeppsson et al. 2007).

3.6 Performance Assessment

3.6.1 Greenhouse Gas Emissions

All emissions are converted to CO₂ equivalent (CO₂e) units, using GWPs of 21 and 310 for CH₄ and N₂O respectively (IPCC 1996), to enable comparison of the magnitude of emissions from each source. The total rate of GHG emission (kg CO₂e/d) attributed to the plant at each time step is calculated using Eq. 3.42. Based on the modelled flow rate, emissions per unit of wastewater treated (kg CO₂e/m³) are also calculated.

$$\begin{aligned} CO2e_{WWTP} = & CO2e_{AS,total} + CO2e_{AD,total} + CO2e_{dewatering} \\ & + CO2e_{energy} + CO2e_{methanol} + CO2e_{effluent} \\ & + CO2e_{sludge} \end{aligned} \quad \text{Eq. 3.42}$$

Average values for performance evaluation can be calculated by rectangular integration, based on the state, duration and flow rate at each time step. This is implemented in the original BSM2 using Eq. 2.19 for flow rate (Q) and Eq. 3.44 for concentrations (Z). The same method is applied during evaluation of emissions in the model developed.

$$\bar{Q} = \left(\sum_{i=245}^{609} Q_i t_i \right) / t_{total} \quad \text{Eq. 3.43}$$

$$\bar{Z} = \left(\sum_{i=245}^{609} Z_i Q_i t_i \right) / \left(\sum_{i=245}^{609} Q_i t_i \right) \quad \text{Eq. 3.44}$$

The contribution of each gas and each emission source is also recorded to enable in-depth investigation into the effects of different control options on GHG production and emission.

3.6.2 Effluent Quality and Legislative Compliance

Effluent quality is assessed using the BSM2 effluent quality index (EQI) (Nopens et al. 2010). This is a weighted sum of effluent pollutant loadings, calculated using Eq. 3.45 (adapted from Alex et al. 2008).

$$EQI = \frac{1}{1000 \cdot t_{obs}} \int_{t_{start}}^{t_{end}} (2 \cdot TSS_e(t) + COD_e(t) + 30 \cdot S_{NKj,e}(t) + 10 \cdot (S_{NO2,e}(t) + S_{NO3,e}(t)) + 2 \cdot BOD_e(t)) Q_e(t) \cdot dt \quad \text{Eq. 3.45}$$

where:

- 1000 = conversion factor [g/kg]
- t_{obs} = Total evaluation time
- TSS_e = effluent TSS [g TSS/m³]
- COD_e = effluent COD [g COD/m³]
- $S_{NKj,e}$ = effluent Kjeldahl nitrogen [g N/m³]
- $S_{NO2,e}$ = Effluent nitrite nitrogen [g N/m³]
- $S_{NO3,e}$ = Effluent nitrate nitrogen [g N/m³]
- BOD_e = Effluent BOD₅ [g BOD/m³]
- Q_e = effluent flow rate [m³/d]

Calculation of effluent TSS, COD, Kjeldahl nitrogen and BOD₅ is as in BSM2. Given additions made to the ASM1 state variables to enable modelling of four-step denitrification and calculation of N₂O emissions, however, nitrate and nitrite nitrogen are now represented by two separate variables ($S_{NO3,e}$ and $S_{NO2,e}$)

instead of the combined ' S_{NO} ' used in ASM1, with nitrogen monoxide (NO) considered separately.

Legislative compliance is assessed with regard to the UWWTD requirements (detailed in Table 3.4 and based on annual mean / 95 percentile values), given that the plant is designed for a 100,000 population equivalent (PE) (Jeppsson et al. 2007). Total phosphorus is not modelled in ASM1 or ASMN and cannot, therefore, be assessed. The number of times that each limit is exceeded during the evaluation is recorded, as well as the total duration of exceedance.

Table 3.4: Requirements for WWTP discharges under the UWWTD (adapted from European Union 1991); total phosphorus and total nitrogen requirements apply only to discharges to sensitive areas

Parameter		Concentration (g/m ³)	Minimum percentage reduction	Absolute maximum concentration (g/m ³)
BOD ₅ without nitrification		25	70-90	50
COD		125	75	250
TSS	2,000-10,000 PE	60	70	150
	>10,000 PE (optional requirement)	35	90	87.5
Total phosphorus	10,000-100,000 PE	2	80	-
	>100,000 PE.	1	80	-
Total nitrogen	10,000-100,000 PE	15	70-80	-
	>100,000 PE	10	70-80	-

3.6.3 Operational Cost

Operational costs are assessed using an operational cost index (OCI), as defined in BSM2 (Nopens et al. 2010), which provides a measure of the average energy demand, energy recovery, carbon source dosage and sludge production for disposal:

$$OCI = AE + PE + 3 \cdot SP + 3 \cdot EC + ME - 6 \cdot MP + HE^{net} \quad \text{Eq. 3.46}$$

where:

AE	=	Aeration energy [kWh/d]
PE	=	Pumping energy [kWh/d]
SP	=	Sludge production for disposal [kg TSS/d]
EC	=	External carbon addition [kg COD/d]
ME	=	Mixing energy [kWh/d]
MP	=	CH ₄ production [kg CH ₄ /d]
HE^{net}	=	Net heating energy for anaerobic digester [kWh/d]

3.7 Wastewater Treatment Plant Control Strategy Modelling

3.7.1 Available Control Handles

Control handles available in BSM2 and their corresponding minimum and maximum allowable values, as specified in the BSM2 code, are listed in Table 3.5.

Table 3.5: Feasible range of available control handles

Control handle	BSM2 Notation	Values		
		Min	Default	Max
Internal recirculation flow rate (m ³ /d)	Q_{intr}	0	61,944	103,240
Return sludge flow rate (m ³ /d)	Q_r	0	20,648	41,296
Wastage flow rate (m ³ /d)	Q_w	0	300	2064.8
Reject water flow rate (m ³ /d)	$Q_{storage}$	0	0	1500
Reactor 1 aeration intensity (d ⁻¹)	KLa_1	0	0	240
Reactor 2 aeration intensity (d ⁻¹)	KLa_2	0	0	240
Reactor 3 aeration intensity (d ⁻¹)	KLa_3	0	120	240
Reactor 4 aeration intensity (d ⁻¹)	KLa_4	0	120	240
Reactor 5 aeration intensity (d ⁻¹)	KLa_5	0	60	240
Reactor 1 carbon source addition (m ³ /d)	$carb_1$	0	2	5
Reactor 2 carbon source addition (m ³ /d)	$carb_2$	0	0	5
Reactor 3 carbon source addition (m ³ /d)	$carb_3$	0	0	5
Reactor 4 carbon source addition (m ³ /d)	$carb_4$	0	0	5
Reactor 5 carbon source addition (m ³ /d)	$carb_5$	0	0	5

3.7.2 Base Case Control Strategies

In order to provide a benchmark against which the performance of newly developed control options can be assessed, the default BSM2 open loop case

and default control strategy are used. A brief overview of the two control strategies is provided below, based upon the detailed description given by Nopens et al. (2010).

The open loop option provides no control actions and control handles are assigned the default values detailed in Table 3.5. Operation of the activated sludge unit is as shown in Figure 3.2.

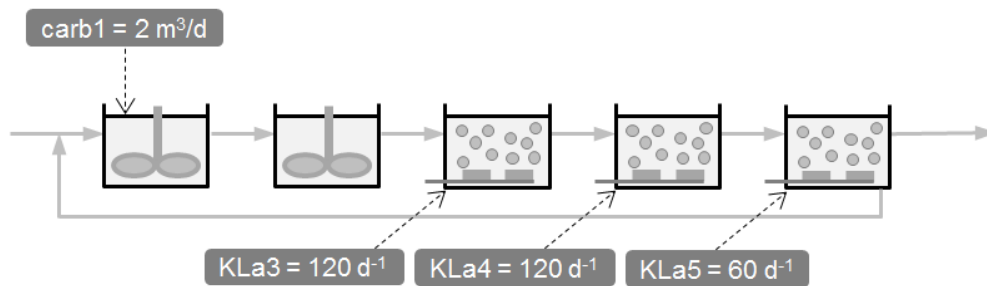


Figure 3.2: Default open loop control of the activated sludge unit

The default closed loop control strategy consists of a DO sensor in reactor 4, a proportional integral (PI) controller and actuators for manipulation of aeration intensities in reactors 3-5, as illustrated in Figure 3.3.

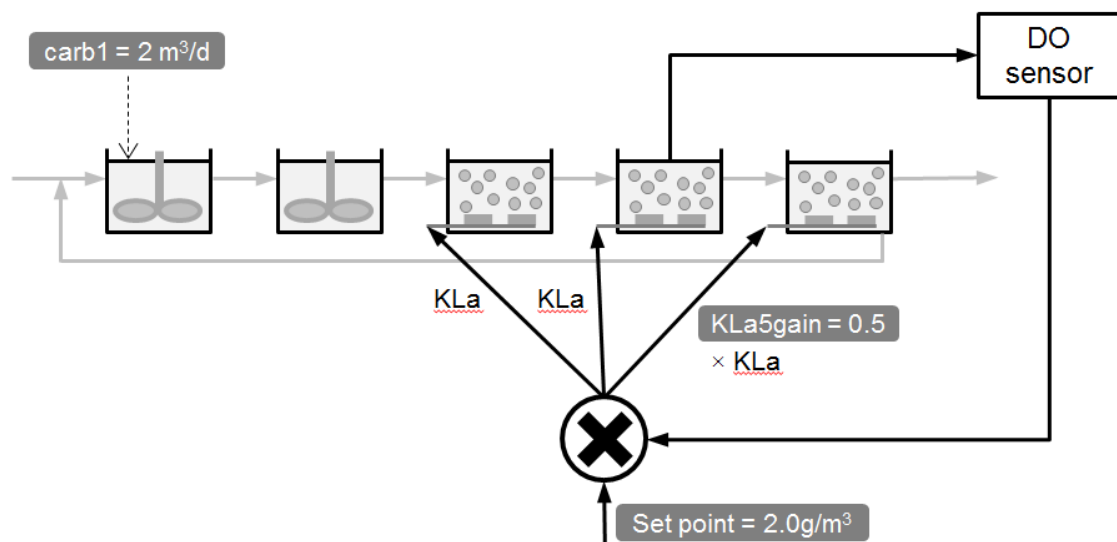


Figure 3.3: Default closed loop control of the activated sludge unit

Control handles not in the aforementioned control loop take the default values prescribed in Table 3.5, with the exception of Q_w which is assigned two different values dependent on the influent wastewater temperature: when the

temperature is below 15°C, a Q_w value of 300 m³/d is assigned, and for the remaining time Q_w is set to 450 m³/d.

Note that this control strategy was not designed to be optimal, nor is it claimed to be – it is simply used as a reference case.

3.7.3 Controllers

Control strategies (including the default closed loop base case and further developments) are implemented using the PI controller model provided in BSM2. PI controllers provide an improvement on proportional control (Eq. 3.47), in which the output is proportional to the error (difference between the measurement and setpoint) and there is an offset (i.e. a difference between the measured variable and the setpoint) at steady state. This problem is rectified by the addition of an integral term (Eq. 3.48), in which all previous errors are summed; this gives a residual value when steady state is reached, allowing offset to be eliminated.

$$u(t) = u_d + \mu(y_s - y(t)) \quad \text{Eq. 3.47}$$

where:

- $u(t)$ = controller output
- u_d = design output (bias)
- μ = constant of proportionality (gain)
- y_s = required value of measured variable (setpoint)
- $y(t)$ = measured variable value

$$u(t) = u_d + \mu(y_s - y(t)) + \frac{\mu}{\tau_i} \int (y_s - y(t)) dt \quad \text{Eq. 3.48}$$

where

- τ_i = reset time of controller (integral time constant)

Tuning parameters for which appropriate values must be selected include the gain and the integral time constant. Increasing the gain results in a faster response but can result in the system becoming unstable. The integral time constant is used to allow independent adjustment of the integral term, with a small value giving in a larger weighting. An insufficient weighting will result in

asymptotic tracking whereas an excessive weighting will yield an oscillatory response.

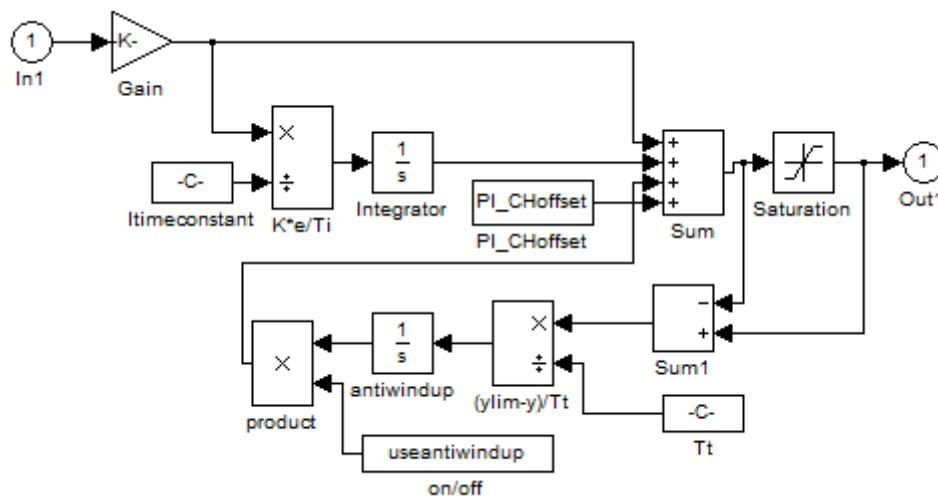


Figure 3.4: Simulink implementation of a PI controller with anti-windup in BSM2

3.8 Base Case Greenhouse Gas Emissions – Example Model Outputs

Examples of emission data extracted from the model running base case open loop simulation with default parameters and the BSM2 default closed loop control strategy (detailed in Section 3.7.2) are shown in Figure 3.5 and Figure 3.6. Figure 3.5 provides a breakdown of mean emissions of each gas and from each source during the one-year evaluation period, whilst Figure 3.6 provides a snapshot of dynamic direct and indirect emissions under each control strategy.

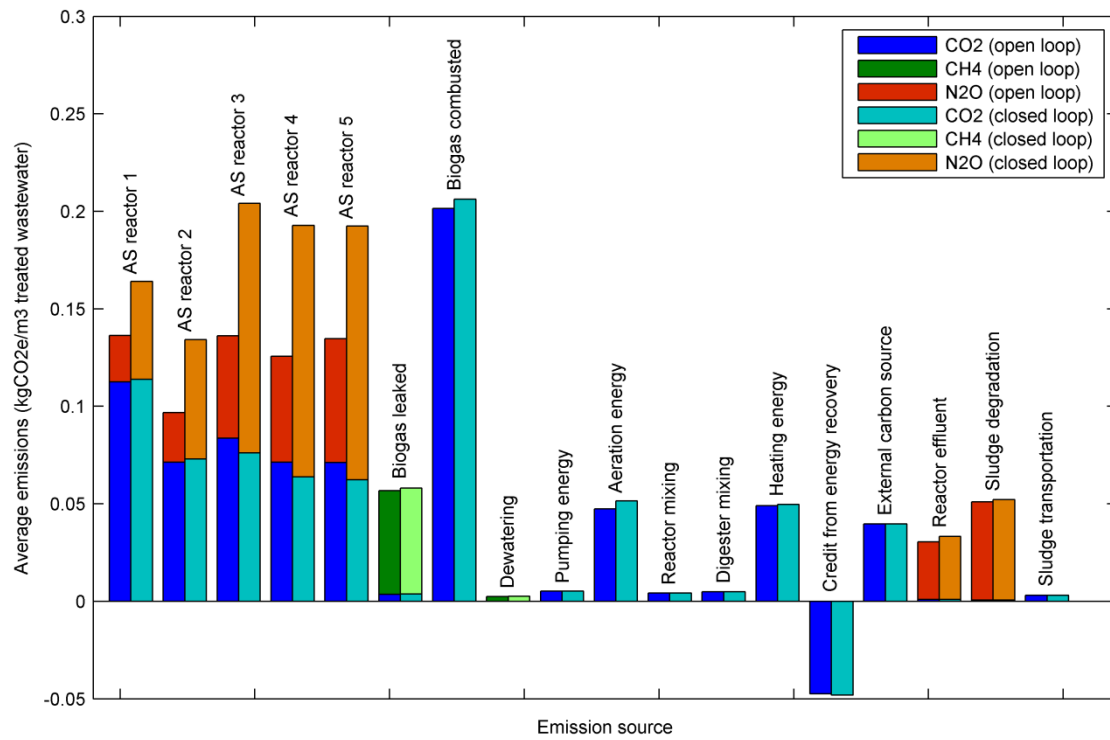


Figure 3.5: Comparison of mean emissions of each GHG and from each source under the default BSM2 open loop and closed loop control strategies

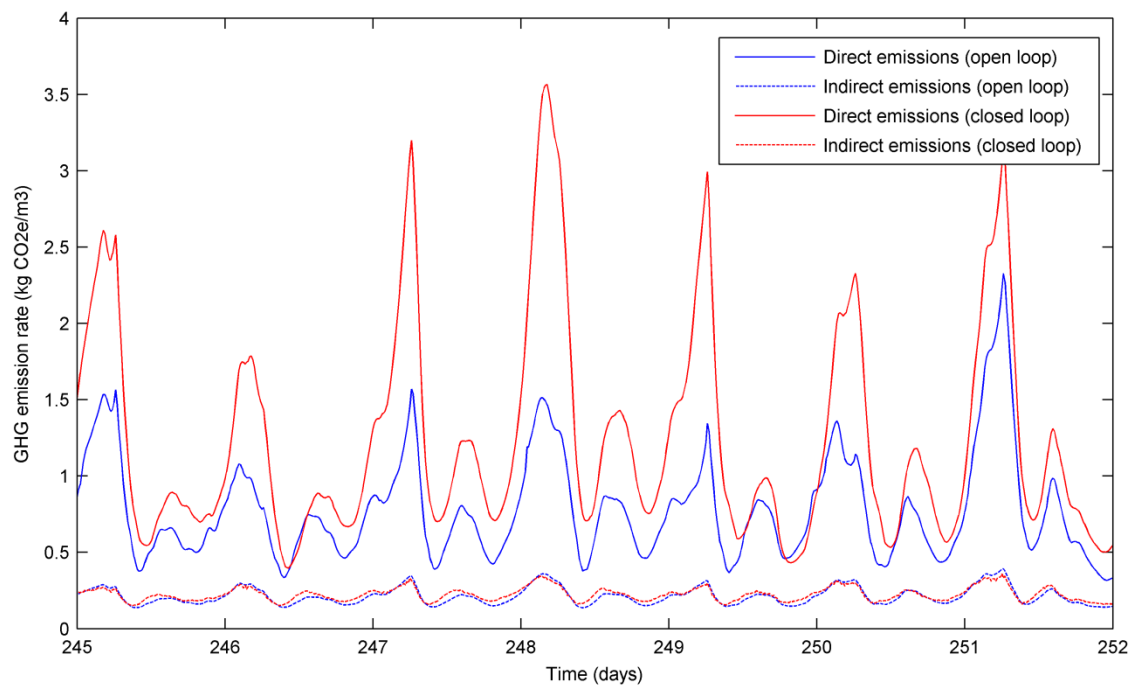


Figure 3.6: Comparison of dynamic direct and indirect emissions per unit of wastewater treated under the default BSM2 open loop and closed loop control strategies (first week of plant evaluation)

It is shown that the default closed loop control strategy, which was developed to improve effluent quality, results in significantly higher GHG emissions than the open loop control strategy, highlighting the importance of taking into account the effect on GHG emissions when adjusting WWTP control. The model outputs also enable identification of the key sources of increased emissions, and it is shown in this example that the increase in total emissions under the closed loop control strategy can be attributed predominantly to an increase in N_2O emissions from the activated sludge reactors. Analysis of dynamic emissions can provide further insight, in this instance showing that direct emissions under the default closed loop control strategy are not consistently worse than those from the open loop case, but contain significantly higher peaks.

3.9 Model Verification

The magnitude of GHG emissions per unit of treated wastewater reported in the literature differs significantly, even for WWTPs with the same or similar treatment processes and control. Total emissions in the range 19,554 – 22,920 kg $\text{CO}_2\text{e/d}$ (equivalent to 0.947 – 1.110 kg $\text{CO}_2\text{e/m}^3$, based on specified flow rate) were reported by Corominas et al. (2012) in an investigation into the effects of different GHG modelling approaches for the BSM2 plant. The BSM2-e emissions model gives total GHG emissions of 1.077 kg $\text{CO}_2\text{e/m}^3$ when using the default BSM2 evaluation period, which is within this range.

It is also important that effluent quality performance indicators simulated in BSM2-e, are comparable with those derived using BSM2. A comparison of the modelled effluent total nitrogen, COD, ammonia and ammonium nitrogen, TSS and BOD_5 under the default closed loop control strategy in BSM2 and BSM2-e is given in Figure 3.7. For clarity, only the first week of the evaluation period is shown.

The most significant difference between the model outputs is in the nitrogen related indicators, where BSM2-e yields consistently higher concentrations but follows the same pattern. Over the 364 day evaluation period, BOD_5 , COD and TSS 95 percentile values differ from those modelled in BSM2 by up to 2.6%, whereas the mean total nitrogen increases by 5.8%. An overview of the percentage change in mean operational cost and effluent quality performance indicator values with respect to those derived in BSM2 is given in Table 3.6.

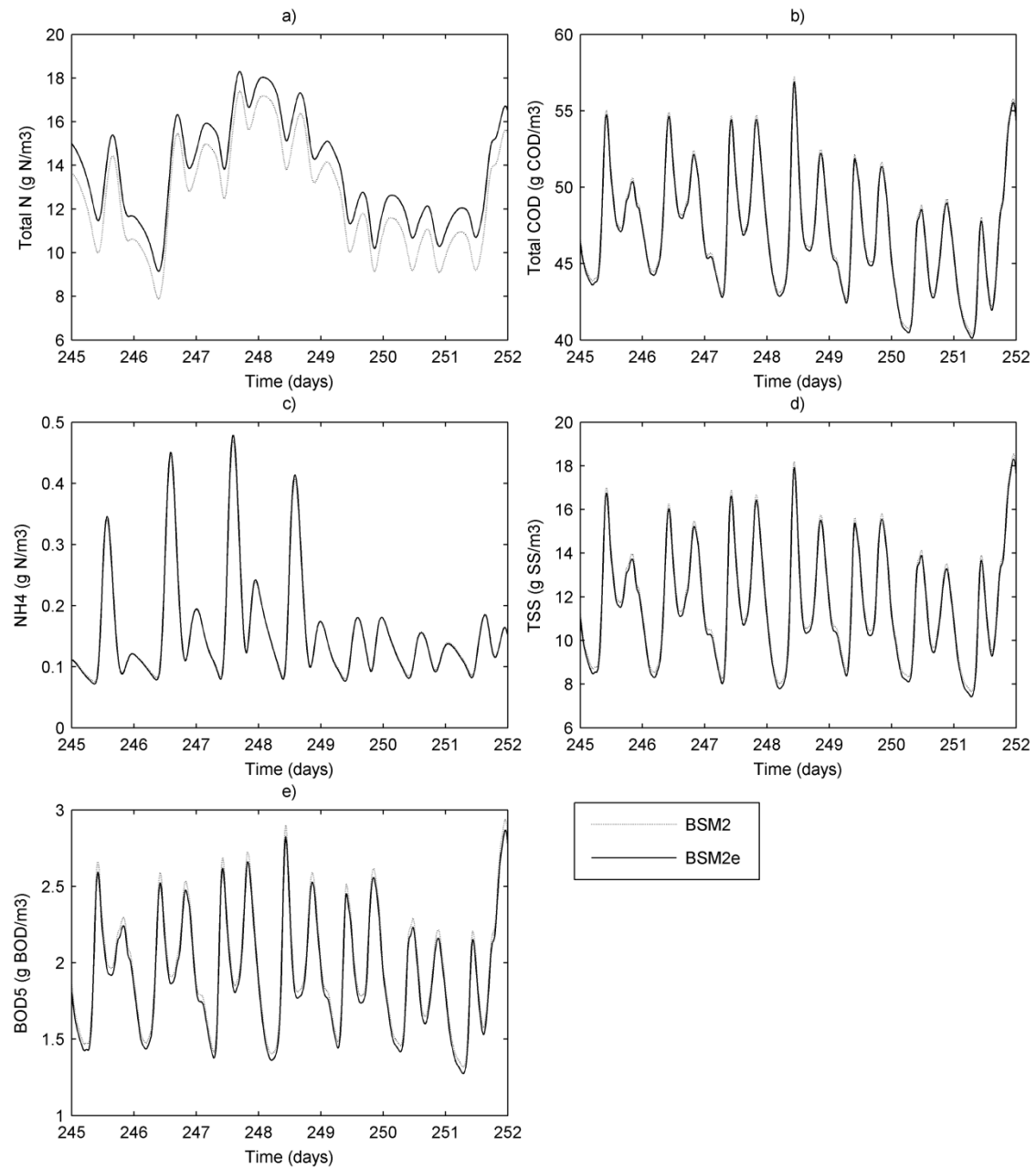


Figure 3.7: Comparison of effluent quality modelled in BSM2-e and BSM2 under the default closed loop control strategy: a) total nitrogen, b) total COD, c) ammonia and ammonium nitrogen, d) TSS, e) BOD₅

Table 3.6: Mean percentage deviation in performance indicators modelled in BSM2-e under the default closed loop control strategy with respect to BSM2

Performance indicator	Percentage change [%]
EQI	2.6
OCI	0.2
BOD ₅ 95 percentile	-2.6
COD 95 percentile	-0.7
TSS 95 percentile	-1.5
Total nitrogen mean	5.8

It is not unexpected that the most significant discrepancy between results from BSM2 and BSM2-e is in the nitrogen components, given that the only alterations in the biological process model are those made to enable calculation of four-step denitrification. These are carried out in accordance with Samie et al. (2011) and using the default parameter values recommended based on Hiatt and Grady (2008). Calibrated values provided by Samie et al. (2011) were tested but resulted in further elevated effluent concentrations since they were derived for modelling of a real, case study plant. Further adjustment of the parameters added for modelling of four-step denitrification is not investigated in this research given that the model is of a hypothetical plant without any data for calibration. As such, the model results should not be taken as definitive and are not purported to provide an entirely accurate evaluation of effluent quality; however, they can still be used to assess relative performance of different control options, enabling identification of general trends and solutions which contribute to improved performance.

4 IDENTIFYING KEY SOURCES OF UNCERTAINTY IN THE MODELLING OF GREENHOUSE GAS EMISSIONS FROM WASTEWATER TREATMENT

4.1 Introduction

Models used to estimate the magnitude of GHG emissions from WWTPs for inventories typically utilise empirical emission factors (e.g. IPCC 2006b), based on the volume of wastewater treated, influent concentrations, effluent concentrations or the mass of wastewater components removed. These emission factors, however, have a high degree of variability and uncertainty (Corominas et al. 2012): for example, N₂O emissions in the range 0 - 90% of the nitrogen-load were reported by Kampschreur et al. (2009). As such, there has been increasing interest in the use of comprehensive process models and mechanistic models to estimate dynamic GHG emissions. Resulting from this, it has been highlighted that significant variability can occur in GHG emissions from WWTPs with different designs (Shahabadi et al. 2009) and operating under different conditions (Flores-Alsina et al. 2011).

As wastewater utilities face the challenge of simultaneously reducing GHG emissions and improving treatment standards due to increasing regulatory pressures, the importance of including GHG emissions in addition to effluent quality and operational costs when evaluating design alternatives is clear. It has been shown that use of automatic control can reduce GHG emissions (Corominas et al. 2010), but models used are typically of hypothetical WWTPs and their results are not always validated with real data (e.g. Hiatt and Grady 2008, Guo et al. 2012b). As such, results are likely to be subject to a high degree of uncertainty; and careful calibration is therefore essential if applying the models and estimation methodologies to a real WWTP for plant design or control strategy development to reduce GHG emissions. Identification of the most significant sources of uncertainty could aid efficient calibration of models and reduce the complexity of future uncertainty analyses, yet there has been little research into the magnitude of uncertainty in GHG emission estimates resulting from uncertainty in model parameters and emission factors.

Sensitivity analysis is a useful tool for identification of the key parameters controlling model outputs (Tang et al. 2007a). However, whilst sensitivity

analyses of dynamic WWTP models have previously been undertaken to investigate the effects of uncertainty in model parameters (e.g. Pons et al. 2008, Flores-Alsina et al. 2009, Ramin et al. 2012), design and operational parameters (Benedetti et al. 2008, Pons et al. 2008) and influent characteristics (Pons et al. 2008), no detailed analyses for identification of key parameters affecting GHG emissions have been carried out. Gori et al. (2011) completed a sensitivity analysis to investigate the effects of varying the pCOD/VSS ratio on the rate of GHG emissions from different sources, but no other model parameters were considered. GSAs of the BSM1 (Sin et al. 2011) and BSM2 (Benedetti et al. 2008), based on Monte Carlo experiments and linear regression, enabled the identification of individual parameters with significant effects on effluent quality and operational cost, but did not consider GHG emissions. However, interactions were not investigated and output uncertainty was attributed to individual parameters only.

The aim of this chapter is to identify individual parameters and parameter interactions which contribute significantly to uncertainty in modelled GHG emissions from wastewater treatment, as well as the more widely used performance indicators of effluent quality and operational cost. Investigation of the relative contributions of specific parameter interactions to output uncertainty represents an advance in WWTP modelling, as previous analyses have not enabled identification of significant interactions. Sensitivity analysis of BSM2-e is carried out using the OAT method, to identify significant individual (first order) effects and inform the selection of parameters for inclusion in further analysis. GSA is then carried out using a variance-based method – Sobol's method (Saltelli 2002) - to investigate higher order effects (interactions). This tool has not, as of yet, been extensively used in wastewater treatment, but previous applications have revealed situations and modelling scenarios in which calibration is likely to be most challenging due to the greater presence of parameter interactions (Massmann and Holzmann 2012) and improved the efficiency of multi-objective optimisation problems by identifying important decision variable interactions (Fu et al. 2012). The results enable identification of: a) parameters that have negligible impact on uncertainty in key model outputs and can, therefore, be excluded from future uncertainty analyses; and b) parameters which contribute significantly to variance in any key model

output, due to first or higher order effects, and so need to be accurately defined for model calibration and application.

4.2 Simulation Strategy and Performance Assessment

The performance of control strategies in BSM2 is typically assessed using a 609 day simulation with predefined dynamic influent data, incorporating stabilisation and evaluation periods, and with initial values determined by simulation with 200 days of constant influent data (as detailed in Section 3.5). This approach is used for OAT sensitivity analysis. In order to carry out a GSA of model parameters, however, it is necessary to significantly reduce the computational demand. Based on analysis of the effects of modifications in stabilisation and evaluation periods on the OAT sensitivity analysis parameter rankings, a reduced dynamic simulation period (consisting of 14 days stabilisation and 14 days evaluation, using days 322-350 of the BSM2 dynamic influent data) has been selected to follow the 200 day steady state initialisation. Whilst this shortened simulation does not reproduce the model outputs obtained with full length stabilisation and evaluation, it has been found to be suitable for assessment of the relative importance of parameters, enabling correct identification of the most sensitive model parameters in OAT sensitivity analysis and resulting in an average change in rank of just 1.1 for all 70 parameters across the three key outputs when compared with analysis using the full dynamic simulation period (609 days).

Performance indicators used include the EQI, OCI and average GHG emissions per unit of wastewater treated. The contribution of each gas and direct and indirect emissions to total GHG emissions are modelled to allow a more in-depth investigation into the most significant sources of uncertainty.

4.3 Sensitivity Analysis Methodology

153 BSM2 parameters are used in the model (excluding those relating to the plant design and operation), and a further 64 are used for the incorporated denitrification and emissions modelling. Given the large number of evaluations required for GSA, it is not practical to include every parameter. Therefore, OAT sensitivity analysis, which requires significantly fewer model evaluations, is used to provide an indication of the importance of each parameter and identify parameters with negligible effect on uncertainty in model outputs.

OAT sensitivity analysis enables changes in model outputs to be clearly attributed to a specific parameter, with no ambiguity, but does not explore the effects of varying two or more parameters simultaneously and is unable to identify any significant interactions. As such, it is followed by GSA to obtain an understanding of second (and higher) order effects and allow exploration of the full parameter space.

4.3.1 Parameter Screening

Parameter Selection and Definitions

Selection of BSM2 parameters is guided by the results of previous GSA by Benedetti et al. (2008): those identified as being not significant for EQI, OCI and effluent NH_4 violations in terms of both the standard regression coefficient and the partial correlation coefficient are excluded from this analysis. Henry's law coefficients used to model dissolution and stripping of CO_2 and CH_4 in the anaerobic digester, however, are added to the analysis, as they may affect emissions despite not having significant effects on previously considered model outputs.

All half-saturation constants added for the modelling of nitrogen conversions are included in the sensitivity analysis, because these parameters have a high degree of uncertainty (Reichert and Vanrolleghem 2001) and affect modelled N_2O production, which has been shown to be a major contributor to GHG emissions from WWTPs (Rodriguez-Garcia et al. 2012). Also, other half-saturation constants were found to be significant by Benedetti et al. (2008).

It is assumed that median values for each parameter are equal to the BSM2 default values (where applicable). For all other parameters, median values are assumed to be those reported in the literature on which the calculations are based. Parameters for which no feasible range is specified in the literature are classified according to the system defined by Reichert and Vanrolleghem (2001) (summarised in Table 4.1) and adopted in later sensitivity and uncertainty analyses (Rousseau et al. 2001, Benedetti et al. 2008).

Table 4.1: Parameter uncertainty classes

Class	Description	Uncertainty (%)	Examples
1	Accurately known parameters	5	External and input parameters, e.g. stoichiometric conversion factors
2	Intermediate	20	Growth rates; temperature dependence coefficients
3	Very poorly known parameters	50	Kinetic parameters, except those listed in Class 2; half-saturation concentrations; specific death and respiration rates

Full details of parameters selected for screening are given in Table 4.2 and Table 4.3. Parameters 1-26 are BSM2 parameters, 27-39 are nitrogen conversion modelling parameters and 40-70 are emissions modelling parameters.

Table 4.2: BSM2 and nitrogen modelling parameters selected for sensitivity analysis screening and GSA (highlighted); HSC = half saturation coefficient

Parameter number/name	Description	Default value		Class	Bounds		Ref.
		Value	Ref.		Lower	Upper	
1/Y_H	Heterotrophic biomass yield (g COD/g COD)	0.67	a	1	0.6365	0.7035	c
2/f_P	Fraction of biomass yielding particulate products	0.08	b	1	0.076	0.084	c
3/i_XB	Biomass nitrogen/COD mass ratio (g N/g COD)	0.08	a	1	0.076	0.084	c
4/mu_H	Heterotrophic max specific growth rate (/d)	4	a	2	3.2	4.8	c
5/K_OH	Oxygen HSC for heterotrophic biomass (g(-COD)/m ³)	0.2	a	3	0.1	0.3	c
6/ny_g	Correction factor for anoxic heterotroph growth	0.8	a	2	0.64	0.96	c
7/ny_h	Correction factor for anoxic hydrolysis	0.8	a	2	0.64	0.96	N/A
8/k_h	Max specific hydrolysis rate (g COD/g COD/d)	3	a	3	1.5	4.5	N/A
9/K_X	HSC of slowly biodegradable substrate (g COD/g COD)	0.1	a	3	0.05	0.15	N/A
10/mu_A	Autotrophic max specific growth rate (/d)	0.5	a	2	0.4	0.6	c
11/K_NH	Ammonia HSC for autotrophs (g NH ₃ -N/m ³)	1	a	3	0.5	1.5	c
12/b_A	Decay coefficient for autotrophic biomass (/d)	0.05	a	3	0.025	0.075	N/A
13/K_OA	Oxygen HSC for autotrophic biomass (g (-COD)/m ³)	0.4	a	3	0.2	0.6	c
14/k_a	Ammonification rate (m ³ /g COD/d)	0.05	a	3	0.025	0.075	N/A
15/F_TSS_CO D	TSS fraction of total COD (g TSS/g COD)	0.75	a	1	0.7125	0.7875	N/A
16/k_hyd_ch	Hydrolysis influence coefficient for carbohydrates (/d)	10	a	N/A	6.25	12.5	Derived from c
17/k_hyd_pr	Hydrolysis influence coefficient for proteins (/d)	10	a	N/A	6.36	13.64	Derived from c
18/k_hyd_li	Hydrolysis influence coefficient for lipids (/d)	10	a	N/A	6.36	13.64	Derived from c
19/K_S_ac	Monod HSC for acetate (kg COD/m ³)	0.15	a	3	0.075	0.225	N/A
20/K_H_co2	Henry's law coefficient for CO ₂ (M _{liq} /bar)	0.035	a	2	0.028	0.042	N/A
21/K_H_ch4	Henry's law coefficient for CH ₄ (M _{liq} /bar)	0.0014	a	2	0.00112	0.00168	N/A
22/frxs_adm	Anaerobically degradable fraction biomass	0.68	a	1	0.646	0.714	N/A
23/v0	Maximum Vesilind settling velocity (m/d)	474	a	2	379.2	568.8	c
24/r_h	Hindered zone settling parameter (m ³ /g SS)	5.76E-04	a	2	0.00046	0.00069	c
25/r_p	Flocculent zone settling parameter (m ³ /g SS)	0.00286	a	2	0.00229	0.00343	c
26/f_ns	Non-settleable fraction	0.00228	a	2	0.00182	0.00274	c
27/K_S2	HSC for S_S for NO ₃ ⁻ reduction (g COD/m ³)	20	d	3	10	30	N/A
28/K_S3	HSC for S_S for NO ₂ ⁻ reduction (g COD/m ³)	20	d	3	10	30	N/A
29/K_S4	HSC for S_S for NO reduction (g COD/m ³)	20	d	3	10	30	N/A
30/K_S5	HSC for S_S for N ₂ O- reduction (g COD/m ³)	40	d	3	20	60	N/A
31/K_NO3	HSC for SNO ₃ for heterotrophs (g N/m ³)	0.2	d	3	0.1	0.3	N/A
32/K_NO2	HSC for SNO ₂ for heterotrophs (g N/m ³)	0.2	d	3	0.1	0.3	N/A
33/K_NO	HSC for SNO for heterotrophs (g N/m ³)	0.05	d	3	0.025	0.075	N/A
34/K_N2O	HSC for SN ₂ O for heterotrophs (g N/m ³)	0.05	d	3	0.025	0.075	N/A
35/ny_g2	Anoxic growth factor for NO ₃ ⁻ reduction	0.28	d	2	0.224	0.336	N/A
36/ny_g3	Anoxic growth factor for NO ₂ ⁻ reduction	0.16	d	2	0.128	0.192	N/A
37/ny_g4	Anoxic growth factor for NO reduction	0.35	d	2	0.28	0.42	N/A
38/ny_g5	Anoxic growth factor for N ₂ O reduction	0.35	d	2	0.28	0.42	N/A
39/ny_Y	Anoxic yield factor for heterotrophs	0.9	d	1	0.855	0.945	N/A

^aAlex et al. (2008)

^bHenze et al. (1987)

^cBenedetti et al. (2008)

^dHiatt and Grady (2008)

Table 4.3: Emissions modelling parameters selected for sensitivity analysis screening and GSA (highlighted); EF = emission factor

Parameter number/name	Description	Default value		Class	Bounds		
		Value	Ref.		Lower	Upper	Ref.
40/f	Ratio of BOD ₅ to BOD _u (g BOD ₅ /g BOD _u)	0.68	e	Class	0.646	0.714	N/A
41/EF_AerOxi	EF for aerobic oxidation of BOD (kg CO ₂ /kg O ₂)	1.1	e	1	1.045	1.155	N/A
42/EF_AerAutoOxi	EF for endogenous respiration of VSS (kg CO ₂ /kg VSS)	1.947	e	1	1.850	2.044	N/A
43/EF_CO2denitWCarb	EF for CO ₂ emissions from denitrification with external carbon source (g CO ₂ /g N ₂ -N)	2.62	Derived from f	1	2.489	2.751	N/A
44/EF_CO2denitWOCarb	EF for CO ₂ emissions from denitrification without external carbon source (g CO ₂ /g N ₂ -N)	2.83	Derived from f	1	2.689	2.972	N/A
45/K_H_n2o_base	Henry's law constant for N ₂ O (mol/l/bar)	0.025	g	2	0.02	0.03	N/A
46/kLa_n2o	Gas transfer coefficient for N ₂ O (/d)	2	h	3	1	3	N/A
47/pgas_n2o	Partial pressure of N ₂ O in atmosphere (bar)	3.20E-07	i	2	2.56E-07	3.84E-07	N/A
48/EF_AnaerBODremCH4	CH ₄ emissions from anaerobic carbonaceous substrate utilisation (g CH ₄ /g BOD)	0.25	f	1	0.238	0.263	N/A
49/EF_AnaerBODremCO2	CO ₂ emissions from anaerobic carbonaceous substrate utilisation (g CO ₂ /g BOD)	0.27	f	1	0.257	0.284	N/A
50/EF_AnaerVSSdecCH4	CH ₄ emissions from anaerobic biomass decay (g CH ₄ /g VSS)	0.35	f	1	0.333	0.368	N/A
51/EF_AnaerVSSdecCO2	CO ₂ emissions from anaerobic biomass decay (g CO ₂ /g VSS)	0.58	f	1	0.551	0.609	N/A
52/leak_frac	Fraction of biogas leaked	0.05	j	3	0.025	0.075	N/A
53/CH4toCO2_combust	Combustion emission factor (g CO ₂ /g CH ₄)	2.75	e	1	2.613	2.888	N/A
54/CH4_conversioneff	Energy conversion efficiency for heating	0.5	k	2	0.4	0.6	N/A
55/PF_Qintr	Pumping energy factor, internal AS recirculation (kWh/m ³)	0.004	a	2	0.0032	0.0048	N/A
56/PF_Qr	Pumping energy factor, AS sludge recycle (kWh/m ³)	0.008	a	2	0.0064	0.0096	N/A
57/PF_Qw	Pumping energy factor, AS wastage flow (kWh/m ³)	0.05	a	2	0.04	0.06	N/A
58/PF_Qpu	Pumping energy factor, pumped underflow from primary clarifier (kWh/m ³)	0.075	a	2	0.06	0.09	N/A
59/PF_Qtu	Pumping energy factor, pumped underflow from thickener (kWh/m ³)	0.06	a	2	0.048	0.072	N/A
60/PF_Qdo	Pumping energy factor, pumped underflow from dewatering unit (kWh/m ³)	0.004	a	2	0.0032	0.0048	N/A
61/mixenergyunitreac	Energy for activated sludge mixing (kW/m ³)	0.005	a	2	0.004	0.006	N/A
62/mixenergyunitAD	Energy for anaerobic digester mixing (kW/m ³)	0.005	a	2	0.004	0.006	N/A
63/cp	Specific heat capacity for water (Wd/gC)	4.84E-05	a	1	4.60E-05	5.09E-05	N/A
64/O2TransferEff	Aeration oxygen transfer efficiency (kg O ₂ /kWh)	1.80	l	2	1.44	2.16	N/A
65/EF_Elec	EF for electricity generation (kg CO ₂ e/kWh)	0.245	k	2	0.196	0.294	N/A
66/EF_EmbodiedCarb	EF for methanol usage (kg CO ₂ e/kg)	1.54	f	2	1.232	1.848	N/A
67/EF_SludgeTransport	EF for transport of sludge (kg CO ₂ e/tonne)	24	f	2	19.2	28.8	N/A
68/EF_SludgeN2O	EF for sludge applied to managed soils (kg N ₂ O/kg N)	0.016	m	2	0.013	0.019	N/A
69/EF_AerBODremI	EF for carbonaceous BOD removal (kg CO ₂ /kg COD)	0.33	f	1	0.314	0.347	N/A
70/EF_EffN2O	EF for N ₂ O emissions from effluent (kg N ₂ O/kg N)	0.008	n	2	0.006	0.009	N/A

^aAlex et al. (2008)

^eMonteith et al. (2005)

^fShahabadi et al. (2010)

^gLide and Frederiske (1995)

^hSamie et al. (2011)

ⁱEuropean Environment Agency (2011)

^lShahabadi et al. (2009)

^kGori et al. (2011)

^lNopens et al. (2010)

^mIPCC (2006a)

ⁿIPCC (2006b)

One-Factor-at-a-Time Sensitivity Analysis

To carry out OAT sensitivity analysis, a simulation is first conducted with all parameters set at their default values; this represents the base case. Further simulations are carried out with each parameter individually set to its upper and lower bound values in turn, whilst all others are held at their default values. Percentage change in each model output with respect to the base case is calculated for each simulation, to determine which parameters cause the greatest variation in model outputs when individually varied within their feasible range.

4.3.2 Global Sensitivity Analysis

Sobol's method (2001) is selected for GSA despite being computationally expensive, as it enables first, second and higher order effects to be distinguished through the calculation of first, second and total order sensitivity indices for each parameter or parameter pair. It also provides more robust sensitivity rankings and a more detailed description of the impact of individual parameters and their interactions on model performance than other GSA methods such as analysis of variance (Tang et al. 2007b), and requires significantly fewer model evaluations than factorial design given the large number of parameters under investigation.

Sobol's method is variance-based and centres upon the decomposition of total variance in a model output into components resulting from specific parameters and parameter interactions; Sobol's sensitivity indices of different orders are then a measure of the output's sensitivity to each individual parameter or parameter interaction.

The total variance (D) of model outputs, resulting from samples of the feasible parameter space, is decomposed and attributed to specific parameters and their interactions as follows, assuming parameters are independent (Tang et al. 2007b):

$$D = \sum_i D_i + \sum_{i < j} D_{ij} + \sum_{i < j < k} D_{ijk} + \dots + D_{12\dots p} \quad \text{Eq. 4.1}$$

where:

D_i = output variance resulting from the i th parameter

D_{ij} = output variance resulting from interaction between i th and j th parameters

p = total number of parameters

First and second order sensitivity indices S_i and S_{ij} represent the percentage contribution of the i th parameter alone and the interaction between the i th and j th parameters to total variance, respectively; total order index S_{Ti} represents the percentage contribution related to the i th parameter, including the interactions of any order, as defined below:

$$S_i = \frac{D_i}{D} \quad \text{Eq. 4.2}$$

$$S_{ij} = \frac{D_{ij}}{D} \quad \text{Eq. 4.3}$$

$$S_{Ti} = 1 - \frac{D_{\sim i}}{D} \quad \text{Eq. 4.4}$$

where:

$D_{\sim i}$ = output variance resulting from all parameters except i th parameter

A high first order sensitivity index indicates a parameter whose individual uncertainty provides a large contribution to output variance, whereas a low first order index and high total order index indicates a parameter whose interactions result in significant output variance, but individually has little effect.

Sobol's method is implemented here as follows:

1. Specify upper and lower bounds of parameters for analysis.
2. Generate $2n$ random parameter samples within the specified bounds, with quasi-Monte Carlo sampling using Sobol's sequence generator.
3. Resample parameters using Saltelli's (2002) extension to Sobol's method, holding one fixed at a time, to generate $n(2p+2)$ parameter sets.
4. Run model with each parameter set in turn, recording values of model outputs.

5. Compute first order, total order and second order sensitivity indices, and rankings for each parameter as detailed by Tang et al. (2007b).
6. Calculate 95% bootstrap confidence intervals for all sensitivity indices.

4.4 One-Factor-at-a-Time Sensitivity Analysis Results and Discussion

OAT sensitivity analysis results are presented in Tornado diagrams, which show the percentage change in each model output with respect to the base case when each model parameter is individually set to its respective upper and lower bounds. Parameters are ranked by the greatest range of percentage change for any model output and results for the most sensitive parameters are presented in Figure 4.1. For clarity, only the 28 parameters with a corresponding range of change of at least 5% in one or more model output are shown.

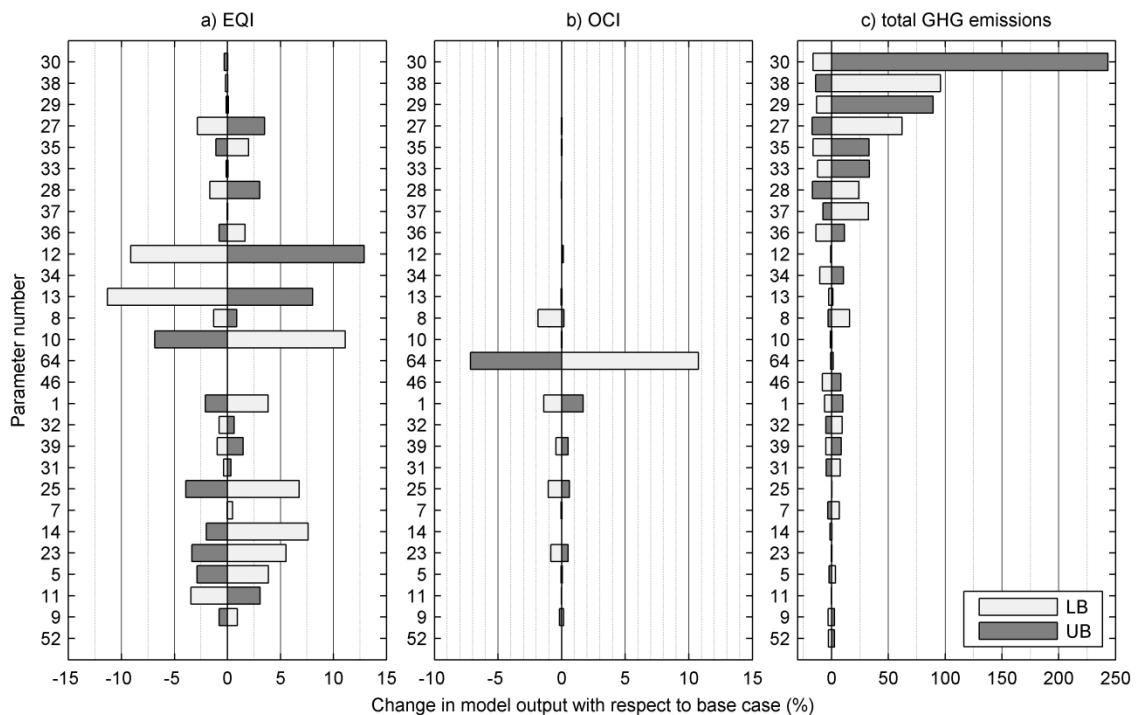


Figure 4.1: Percentage change in model output resulting from variation of individual parameter values. Note the different x-axis scale in c).

Variation of a single parameter within its feasible range can have particularly significant effects on modelled GHG emissions; setting the half saturation constant for readily biodegradable substrate for N_2O reduction (parameter 30) to its upper bound, for example, results in a 244% increase in reported GHG emissions. Individual variation of a further eight parameters is shown to result in a range of at least 25% change in GHG emissions.

A maximum range of variation in total GHG emissions of 260%, resulting from uncertainty in just one parameter (No. 30), is observed, whereas maximum changes in EQI and OCI are significantly lower at 22.0% (No. 12) and 17.9% (No. 64) respectively. This confirms that accurate calibration of the model with regards to GHG emissions modelling is extremely important. The nine parameters shown to have greatest individual effects on GHG emissions are all used in the modelling of nitrogen conversions, suggesting that uncertainty in GHG emissions corresponds primarily to uncertainty in the rate of N_2O production. The three parameters to which GHG emissions are shown to be most sensitive result in negligible change in EQI and OCI and ought, therefore, to be relatively simple to calibrate if significant higher order effects are not identified in GSA and accurate measurements are available.

The greatest changes in EQI arise due to uncertainty in the original BSM2 parameters, and nitrogen modelling parameters have comparatively little impact. Uncertainty in emissions modelling parameters has no effect on EQI. Uncertainty in BSM2 parameters contributes to uncertainty in all three of the key model outputs, although OCI is affected to a lesser degree (maximum 3.2% change, compared with 22.0% and 19.0% for EQI and GHG emissions respectively). It is, therefore, important to take into account the effects of BSM2 parameter values on GHG emissions as well as on conventional performance assessment measures when calibrating the model.

The OCI is affected predominantly by uncertainty in the oxygen transfer efficiency (parameter 64) during OAT sensitivity analysis, suggesting that this is particularly important to consider when carrying out uncertainty analyses with regard to operational costs.

4.5 Sobol's Method Global Sensitivity Analysis Results and Discussion

GSA was carried out using the highlighted parameters in Table 4.2 and Table 4.3, selected based on OAT sensitivity analysis screening results. In addition to the 28 parameters shown in Figure 4.1, these include a further 11 of the highest ranked parameters. First order, second order and total order sensitivity indices computed using a sample size of 4,000 are presented, and parameters are classified as either 'non-influential', 'sensitive' or 'highly sensitive' based on their contribution to output variance. A threshold of 1% contribution to output

variance (i.e. a sensitivity index of at least 0.01) is used to define sensitive parameters, and a 10% contribution (i.e. a sensitivity index of at least 0.1) for highly sensitive parameters.

It is known that small numerical errors can result from the truncation of Monte Carlo approximations used in Sobol's method for calculation of integrals (Tang et al. 2007b), so slightly negative indices are assumed to equal zero. Instances in which the total order index is slightly greater than one or the total order index is less than the sum of the first and second order indices are also attributed to such errors. For the OCI, total order indices sum to less than one; this apparent error, however, is fully accounted for by the 95% confidence intervals.

Bootstrapped confidence intervals, calculated using 1,000 resamples, are presented for all first and total order indices greater than 0.01. It is noted that some sensitivity indices have a high degree of uncertainty, with the greatest confidence interval being 0.501 ± 0.099 . The number of samples generated for analysis was quadrupled from preliminary analyses in an attempt to reduce confidence intervals, but further increase in the number of samples is impractical due to the high computational demand. Large uncertainties are not unexpected for Sobol's method, however, due to random number generation effects (Tang et al. 2007b), and confidence intervals in excess of 20% of the corresponding sensitivity indices have been reported for previous analyses (Tang et al. 2007a, Tang et al. 2007b). Despite large confidence intervals, the sensitivity indices can still be used to provide an indication of the relative significance of uncertainty in each modelling parameter in terms of its effects on model output uncertainties.

4.5.1 Sensitivity Indices Based on EQI, OCI and Total GHG Emissions

First and Total Order Indices

First and total order sensitivities calculated based on EQI, OCI and total GHG emissions are presented in Figure 4.2.

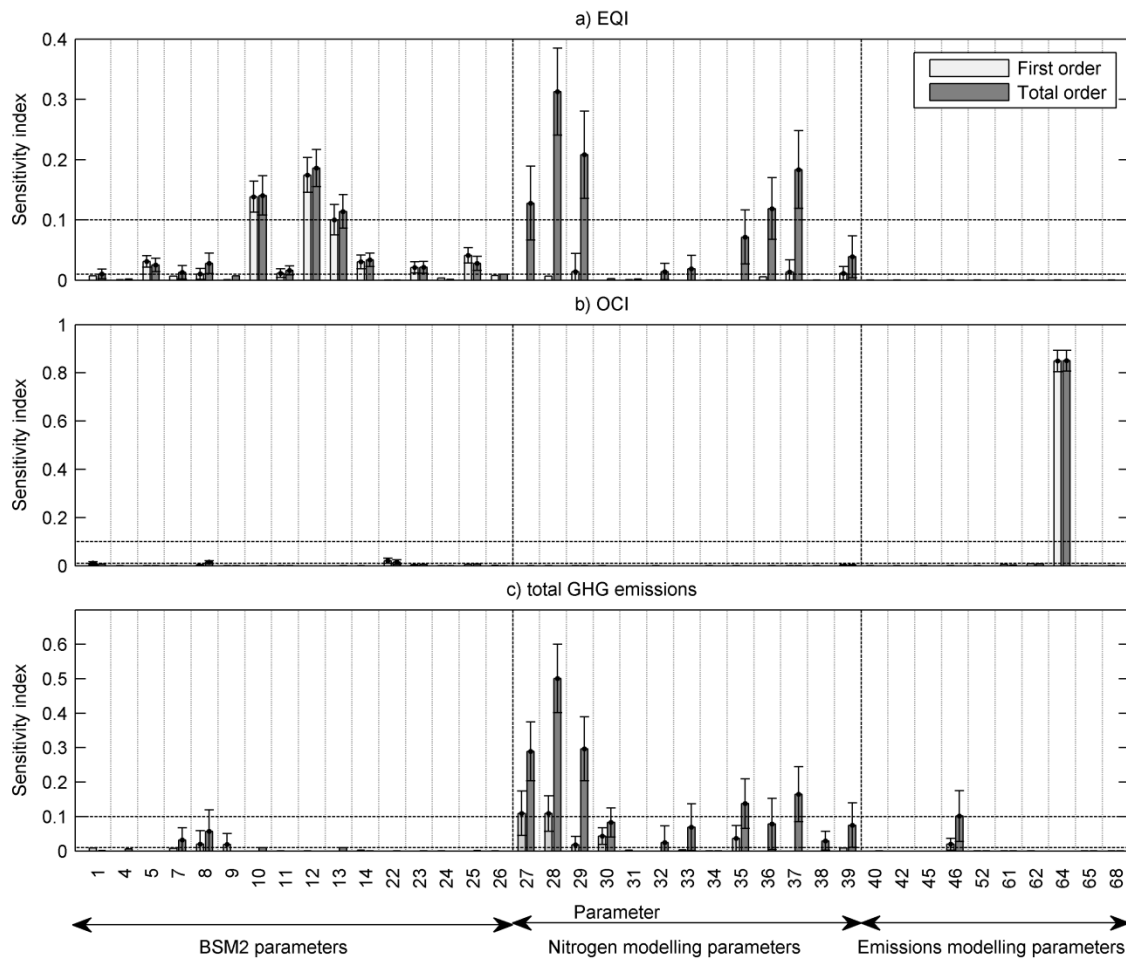


Figure 4.2: First and total order sensitivity indices calculated using Sobol's method, with confidence intervals shown for parameters classified as sensitive or highly sensitive

The EQI is shown to be sensitive or highly sensitive to twenty BSM2 and nitrogen modelling parameters, with emissions modelling parameters (predictably) having no effect. Uncertainty in the BSM2 parameters results primarily in first order effects, but it is shown that higher order effects are dominant for nitrogen modelling parameters, and that some important parameters cannot be identified based on their individual effects alone. For example, OAT sensitivity analysis suggests that EQI is not sensitive to parameters 28 and 29 (ranked 11th and 25th), but investigation into their interactions using Sobol's method shows that they are the greatest contributors to output variance.

The effects of parameter interactions on OCI uncertainty are negligible, and there is only one highly sensitive parameter: the oxygen transfer efficiency

(parameter 64). OCI is also sensitive to three BSM2 parameters, although their contribution to output variance is insignificant in comparison.

All parameters classed as highly sensitive based on GHG emissions are used in the modelling of N₂O production and emission, supporting the earlier suggestion that, due to their high GWP, uncertainty in the rate of N₂O emissions is a significant contributor to uncertainty in total GHG emissions. Variance in modelled GHG emissions is predominantly due to interactions, although first order effects are still significant for some nitrogen modelling parameters: parameter 28, for example, contributes 50.1% of output variance to total output variance, with 10.9% from the parameter itself and 39.2% from its interactions with other parameters. It would, therefore, be beneficial to investigate the effects of specific interactions, to ensure that suitable allowance is made in future analyses and model calibration.

It can be seen that there is only one parameter to which all three key model outputs are sensitive (parameter 8), although both EQI and GHG emissions are highly sensitive to the half saturation coefficients for readily biodegradable substrate for NO₃, NO₂ and NO reduction.

Fourteen parameters are not classed as sensitive based on any of the three key outputs. Whilst it is suggested that these are low priority for future uncertainty analyses, it is noted that the classification of these parameters (and others) will be influenced by the choice of upper and lower bounds for their possible values. If uncertainty in a parameter is greater than considered here, then the parameter may have a greater impact on variance in EQI, OCI and GHG emissions than expected. This may be particularly relevant to parameters such as the biogas leakage fraction (no. 52), which could feasibly be reduced to zero, and the emission factor for electricity generation, which is known to vary greatly (as discussed in Sections 2.1.2 and 3.3.1).

Second Order Indices

Second order sensitivity indices calculated based on output GHG emissions and EQI are presented in Figure 4.3 (second order indices based on OCI are not calculated since it has been shown that the effect of interactions is negligible): the shade of grey represents the sensitivity index magnitude for the corresponding parameter pair. Whilst no interactions due to individual

parameter pairs can be classed as highly sensitive, there are numerous parameter pairs which have a significant impact on output variance in GHG emissions and EQI (index ≥ 0.01 , shown with a circle).

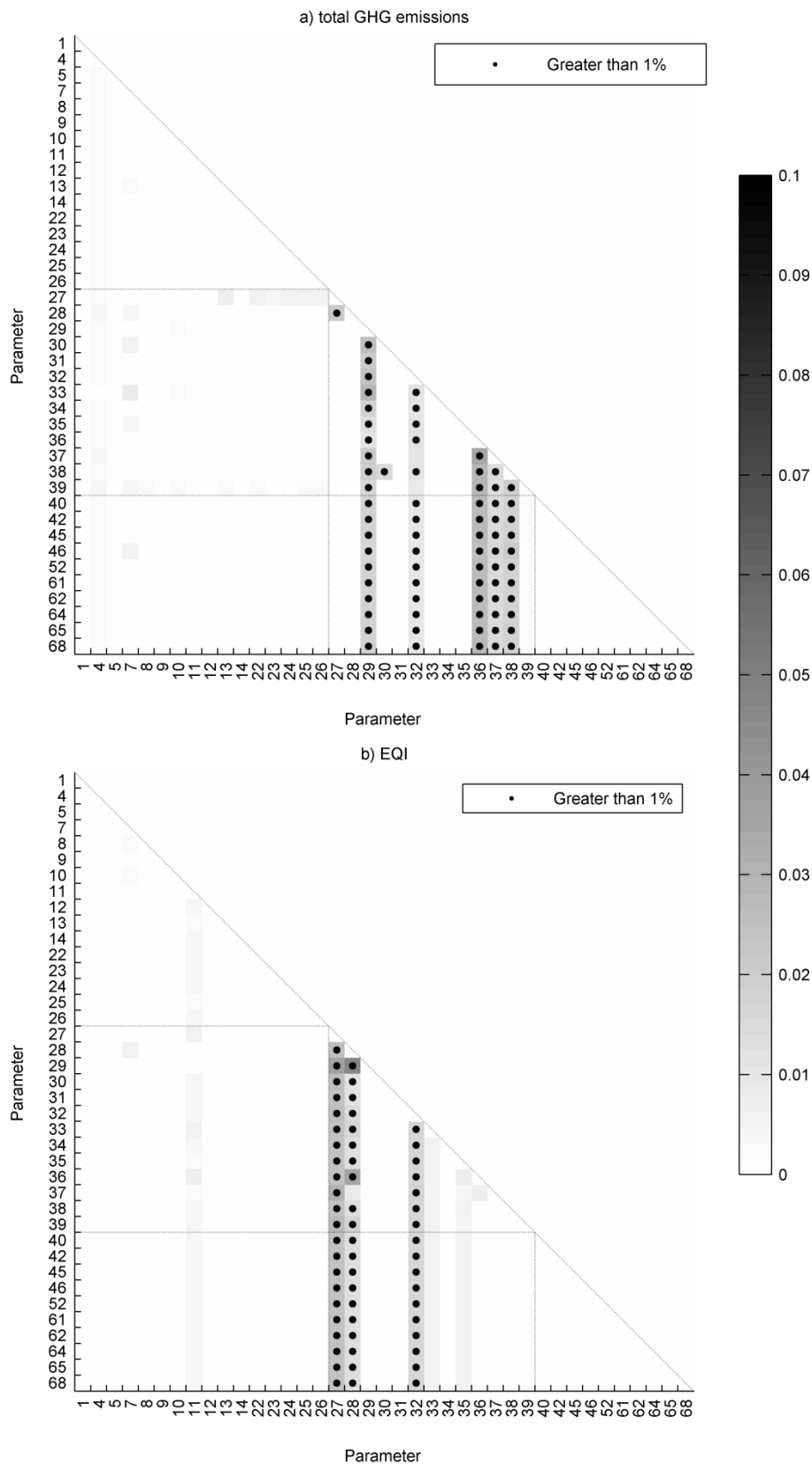


Figure 4.3: Second order sensitivity indices calculated using Sobol's method

Not all parameters identifiable as having significant interactions, based on the difference between their total and first order sensitivity indices, are found to have sensitive parameter pairs, and the second order effects of some parameters account for only a small proportion of total output variance resulting from their interactions. Second order effects involving parameter 28, for example, contribute to 3.1% of variance in total GHG emissions, but all interactions with this parameter contribute 39.2% of output variance, showing that higher order interactions are significant; calibration of such parameters is, therefore, likely to be challenging.

In terms of both GHG emissions and EQI, all sensitive parameter pairings include at least one nitrogen modelling parameter and the most significant second order interactions are between two nitrogen modelling parameters. This provides further support to the earlier suggestion that careful calibration of nitrogen modelling parameters is vital if model output uncertainty is to be reduced.

4.5.2 Sensitivity Indices Based on Component GHG Emissions

Having identified parameters to which total GHG emissions are sensitive, the effects of uncertainty in these parameters on emissions of different gases and from different sources are explored, and the contribution of uncertainty in different emission components to uncertainty in total GHG emissions is investigated.

The characteristics of GHG emissions resulting from the 160,000 parameter sets modelled for GSA are summarised in Table 4.4, from which it can be seen that variance in direct N₂O emissions contributes greatly to variance in total GHG emissions. Indirect emissions provide a comparatively small (12%) contribution to mean total GHG emissions, but are the second greatest contributor to total variance. Variance in direct CO₂ and CH₄ emissions provides negligible contribution to total variance, despite contributing 33% of mean total GHG emissions. This suggests that, unless uncertainty in direct N₂O emissions is significantly reduced by reduction of relevant parameter uncertainties, inclusion of parameters to which only direct CO₂ and CH₄ emissions are sensitive is unnecessary when calculating uncertainty in total GHG emissions.

Further GSA therefore focuses on sources of uncertainty in direct N₂O and total indirect emissions.

Table 4.4: Characteristics of total and component GHG emission results used for Sobol's method sensitivity analysis (emissions per m³ treated wastewater)

	Direct CO ₂	Direct CH ₄	Direct N ₂ O	Total indirect	Total GHGs
Base case (kg CO ₂ e/m ³)	0.4795	0.0595	0.1426	0.1872	0.8688
Mean (kg CO ₂ e/m ³)	0.4736	0.0596	1.1725	0.1913	1.8970
Variance ((kg CO ₂ e/m ³) ²)	0.0006	0.0003	9.6585	0.2047	9.7978

First and total order sensitivity indices based on emission components are presented in Figure 4.4. There is negligible difference between those based on total GHG emissions and those based on direct N₂O emissions only, confirming that reducing uncertainty in N₂O emissions is key to reducing uncertainty in total GHG emissions.

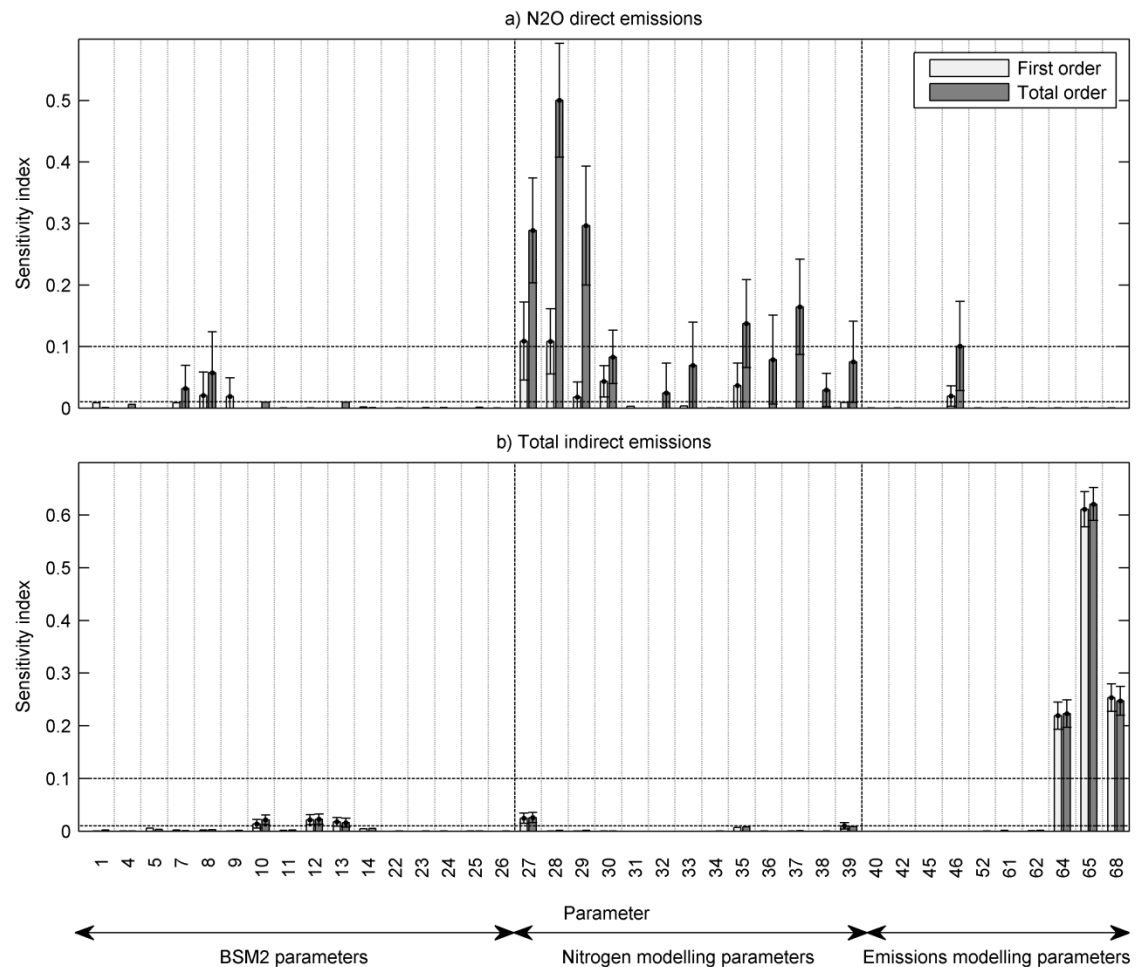


Figure 4.4: First and total order sensitivity indices based on direct N₂O emission and total indirect GHG emissions, with confidence intervals shown for parameters classified as sensitive or highly sensitive

Uncertainty in indirect GHG emissions is primarily attributed to first order effects of the oxygen transfer efficiency and emission factors for carbonaceous BOD removal and N₂O from the WWTP effluent and sludge (parameters 64, 65 and 68). A further five sensitive parameters are also identifiable. Given that the effects of interactions are negligible and the highly sensitive parameters are not classed as sensitive based on any other model output, calibration with regards to indirect emissions ought to be straightforward.

As parameter interactions are shown to contribute significantly to variance in direct N₂O emissions, second order sensitivity indices are calculated and are shown in Figure 4.5. Again, the indices based on direct N₂O emissions are very similar to those based on total GHG emissions, although there are differences: whilst all sensitive parameter pairs still include at least one nitrogen modelling

parameter, nine pairs involving the half saturation coefficient for NO₂ for heterotrophs (parameter 32) are no longer classified as sensitive. This suggests that their second order interactions impact primarily on other GHG emissions. All emissions modelling parameters are involved in significant second order interactions with parameters 29, 36, 37 and 38 and are, therefore, particularly important to reduce uncertainty in and consider simultaneously during calibration. Also important is the interaction between parameters 28 and 27, which alone contributes 2% of variance in direct N₂O emissions.

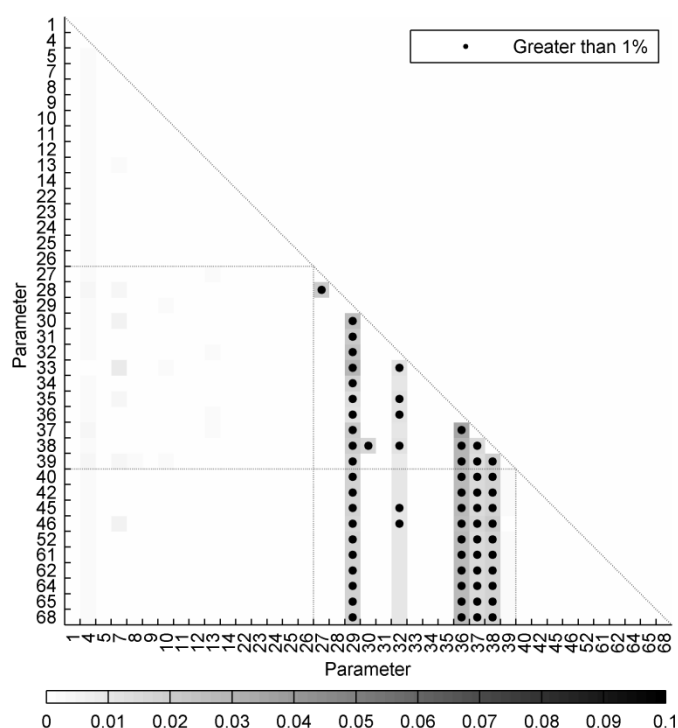


Figure 4.5: Second order sensitivity indices calculated using Sobol's method, based on direct N₂O emissions

4.6 Key Sources of Uncertainty and Comparison of Results

Model parameters to which at least one of the key model outputs (EQI, OCI and total GHG emissions) is sensitive, based on the corresponding sensitivity indices, are detailed in Table 4.5. Shading is used to distinguish sensitive and highly sensitive parameters for each output, and rankings based on OAT sensitivity analysis results as well as first and total order indices are provided. The maximum specific hydrolysis rate (parameter 8) is classified as sensitive based on all three key model outputs, showing that it is necessary to simultaneously consider its impacts on each output during calibration. A further ten parameters are classified as sensitive based on both EQI and GHG

emissions; their effects on both effluent concentrations and GHG emissions must be taken into account during calibration. The remaining fourteen parameters are classified as sensitive based on just one model output.

Table 4.5: Ranking of model parameters to which at least one key model output is sensitive

Parameter number	Sensitivities based on EQI			Sensitivities based on OCI			Sensitivities based on total GHG emissions		
	GSA sensitivity rank		OAT rank	GSA sensitivity rank		OAT rank	GSA sensitivity rank		OAT rank
	First order	Total order		First order	Total order		First order	Total order	
1		20	10						
5	5	14	7						
7		19	25					12	17
8	12	12	17		3	4	6	11	11
10	2	5	3						
11	10	17	8						
12	1	3	1						
13	3	8	2						
14	6	11	5						
22				2	2	2			
23	7	15	6						
25	4	13	4						
27		6	9				1	3	4
28		1	11				2	1	7
29	8	2	25				7	2	3
30							3	7	1
32		18	19					14	14
33		16	30					10	6
35		9	13				4	5	5
36		7	15					8	9
37	9	4	28					4	8
38								13	2
39	11	10	14					9	15
46							5	6	12
64				1	1	1			

Light grey shading denotes sensitive parameters, based on corresponding index

Dark grey shading denotes highly sensitive parameters, based on corresponding index

OAT sensitivity analysis results provide a good indication of the most significant individual sources of uncertainty in output EQI and OCI: parameters classified as highly sensitive based on their first order indices are also the highest ranked in OAT sensitivity analysis. For GHG emissions, however, OAT sensitivity analysis did not enable correct identification of any parameters classified as highly sensitive in GSA and there are significant discrepancies between the first order index rankings and OAT sensitivity analysis rankings for all parameters.

This shows that a full GSA is an important tool even when identification of only significant first order effects is required.

GSA using Sobol's method also enables identification of parameters involved in interactions with significant effects on uncertainty in the model output. As such, highly sensitive parameters have been identified which have comparatively low first order sensitivity indices and contribute to output uncertainty primarily through higher order effects. These are not all identifiable by OAT sensitivity analysis – uncertainty in parameter 28, for example, provides the greatest contribution to uncertainty in output EQI, but is ranked only 11th based on the results of OAT sensitivity analysis. This highlights the importance of including the effects of interactions when identifying and prioritising sources of uncertainty.

4.7 Conclusions

This chapter uses sensitivity analysis tools to assess the contribution of uncertain parameters in the modelling of GHG emissions from wastewater treatment to uncertainty in model outputs, and to identify parameters to which the outputs are most sensitive. Sensitivity analyses are carried out using both the OAT method (also used for screening) and Sobol's method (to enable identification of significant interactions), from which the following conclusions can be drawn:

- Parameters used in the modelling of nitrogen conversions have negligible first order (individual) effects on the EQI and, based on OAT sensitivity analysis, have a low significance rank. Use of Sobol's method, however, enables identification of parameters involved in interactions that contribute greatly to uncertainty in EQI. This highlights the importance of considering parameter interactions using a variance-based GSA method such as Sobol's method.
- Uncertainty in total GHG emissions from the modelled WWTP result primarily from uncertainty in direct N₂O emissions, due to their high GWP. Key sources of uncertainty in direct N₂O emissions include the half saturation coefficients for readily biodegradable substrate for NO₃, NO₂ and NO reduction. As such, further work to reduce uncertainty in these

parameter values would be beneficial in order to reduce uncertainty in total GHG emissions.

- GSA reveals that parameters used in the modelling of nitrogen conversions are key sources of uncertainty in both EQI and total GHG emissions – therefore, when calibrating the model, it is important to consider the effects on both of these outputs.
- Uncertainty in the OCI is shown to be predominantly due to first order effects resulting from uncertainty in the oxygen transfer efficiency. Neither EQI or GHG emissions are sensitive to this parameter, thus calibration of model outputs used in calculation of the OCI is expected to be relatively straightforward if this knowledge is taken into account.

In summary, this chapter has enabled the identification of parameters that contribute significantly to uncertainty in one or more model outputs and require careful calibration, as well as those that provide negligible contribution and are low priority for future uncertainty analyses.

5 IDENTIFYING SENSITIVE SOURCES AND KEY CONTROL HANDLES FOR THE REDUCTION OF GREENHOUSE GAS EMISSIONS

5.1 Introduction

Appropriate operation of wastewater treatment processes can play a significant role in reducing GHG emissions (Gori et al. 2011) and WWTP control strategies which both improve effluent quality and reduce GHG emissions have been developed (Flores-Alsina et al. 2011, Guo et al. 2012b). However, control handles with the greatest impact on GHG emissions need to be identified if significant further improvements are to be made. The effects of adjusting the DO setpoint, SRT (by alteration of the wastage flow rate), carbon source addition rate, primary clarifier TSS removal efficiency, anaerobic digester temperature and control of the digester supernatant return flow on GHG emissions from different sources, as well as effluent quality and operational cost, have been assessed previously (Flores-Alsina et al. 2011, Flores-Alsina et al. 2014). Since the effects of interactions due to simultaneous adjustments or strategy implementations were not considered and variation within the full range of feasible values not explored, however, key findings regarding the effects of these adjustments are of limited use in further control strategy development. The importance of analysing a wide range of values for each control handle is evidenced by the identification of non-linear relationships between parameter values and effluent quality, and control handle values beyond which further increase produces no additional gain (Nopens et al. 2007). Previous analysis (Benedetti et al. 2012) has identified control handles to which effluent quality and operational cost are most sensitive in the BSM2 (Jeppsson et al. 2007), taking into account simultaneous variation across a range of values, but the impacts on GHG emissions have not been considered. Furthermore, whilst the effects of interactions are automatically considered when multiple control changes are implemented, the relative significance of specific interactions between control handles cannot be revealed explicitly to inform control strategy development by focusing on interactions.

It would also be beneficial to investigate variance in GHG emissions from different sources, in order that control strategy development can focus on those with greatest potential for improvement. For example, manufacture of material for on-site usage is a key source of GHG emissions (Shahabadi et al. 2010) but,

given that previous studies show little variation in emissions resulting from chemical consumption under different control strategies (Guo et al. 2012b), attempts to reduce GHG emissions by reduction of carbon source addition may be ineffective without introduction of alternative treatment processes such as Anammox. Conversely, it has been found that implementation of different control strategies can result in significant variation in the magnitude of N_2O emissions from activated sludge (Guo et al. 2012b), suggesting that there is great potential for reduction of total GHG emissions from wastewater treatment by reducing N_2O emissions. It is known that DO concentration and COD/N ratios, which are controlled by adjustment of aeration and carbon source addition rates, play a key role in controlling production of N_2O (Kampschreur et al. 2009, Guo et al. 2012b), yet there is a need to investigate the effects on net emissions of varying these control handles simultaneously, as well as the effluent quality and operational cost. At present, there are conflicting observations regarding the effects of WWTP control on N_2O emissions: Clippeleir et al. (2014), for example, measured increased N_2O emissions when operating with a high DO setpoint, whilst Guo et al. (2012b) found a reduction in DO setpoint to correspond with an increase in N_2O emissions.

This chapter aims to detect control handles to which key performance indicators (including GHG emissions, effluent quality and operational cost) are sensitive and to identify the most significant sources of variance in total GHG emissions, taking into account interaction effects. It is important to identify control handles to which GHG emissions are significantly more sensitive than effluent quality or operational costs, since selection of their values might be attributed little importance in conventional design practices. This knowledge will guide the selection of control handles for efficient and effective control strategy development, based on those with potential to yield the greatest improvements. Knowledge of control handles to which no key model outputs are sensitive will also reduce the number of decision variables required, therefore reducing computational demand and improving the feasibility of multi-objective optimisation for control strategy development.

Sensitivity analysis is employed to identify important parameters controlling model outputs (Tang et al. 2007a); this approach can be utilised to assist system optimisation by detecting the most influential control handle(s)

(Naessens et al. 2012), and has previously been shown to be effective (Fu et al. 2012). Analysis is carried out through the combined use of a local sensitivity method - OAT - and a variance-based global method – Sobol's method; this allows trade-offs to be investigated, and reveals control handles with significant individual effects on GHG emissions, effluent quality and operational cost, as well as those with interaction effects which contribute significantly to variance in the model outputs. Model evaluations carried out with GSA also reveal the most significant sources of variance in GHG emissions and, therefore, the sources from which it is most important to control and monitor GHG emissions.

5.2 Sensitivity Analysis Methodology

5.2.1 Control Handles

Control handles included in this analysis are restricted to 14 available in BSM2 (shown in Figure 5.1): aeration and carbon source addition rates in each of the five reactors ($KLa1-5$ and $carb1-5$), internal recirculation flow rate (Q_{intr}), return sludge flow rate (Q_r), wastage flow rate (Q_w) and reject water flow rate setpoint ($Q_{storage}$). Q_r and Q_w are included despite previously having been found not to have a significant effect on effluent quality and operational cost within the ranges tested (Benedetti et al. 2008), since their interactions with other control handles were not previously investigated, their effects on GHG emissions are unknown, and the range of Q_w values considered was insufficient to encompass those previously proposed for operation of BSM2 (Nopens et al. 2010). It is also known that wastage flow rate affects aeration requirements and sludge production, both of which contribute significantly to operational costs.

Table 5.1: Feasible range of control handles and limits used for sensitivity analysis

Control handle	Notation	Values		
		Lower limit	Default	Upper limit
Internal recirculation flow rate (m ³ /d)	Qintr	51,620	61,944	72,265
Return sludge flow rate (m ³ /d)	Qr	16,518	20,648	24,778
Wastage flow rate (m ³ /d)	Qw	93.5	300	506.5
Reject water flow rate set point (m ³ /d)	Qstorage	0	0	150
Reactor 1 aeration intensity (d ⁻¹)	KLa1	0	0	24
Reactor 2 aeration intensity (d ⁻¹)	KLa2	0	0	24
Reactor 3 aeration intensity (d ⁻¹)	KLa3	96	120	144
Reactor 4 aeration intensity (d ⁻¹)	KLa4	96	120	144
Reactor 5 aeration intensity (d ⁻¹)	KLa5	36	60	84
Reactor 1 carbon source addition (m ³ /d)	carb1	1.5	2	2.5
Reactor 2 carbon source addition (m ³ /d)	carb2	0	0	0.5
Reactor 3 carbon source addition (m ³ /d)	carb3	0	0	0.5
Reactor 4 carbon source addition (m ³ /d)	carb4	0	0	0.5
Reactor 5 carbon source addition (m ³ /d)	carb5	0	0	0.5

5.2.2 Preliminary Analysis

Preliminary investigation is carried out using OAT sensitivity analysis, which allows changes in model outputs to be attributed to a specific control handle, with no ambiguity: two WWTP performance evaluations are carried out for each control handle (one with the value at its lower bound and another with the value at its upper bound, whilst all other control handles are held at their default value) and the percentage change in each model output with respect to the base case is calculated. The results are then used to identify control handles with the highest control authority, and to determine the direction of change in each model output resulting from an increase or decrease in control handle value.

Upper and lower bound model outputs (Y) for control handle i are calculated using Eq. 5.2 and Eq. 5.3 respectively, where n is the number of control handles, x is the control handle value and x_{-i} denotes the value of all control handles except x_i .

$$Y_{base} = f(x_{1,base...n,base}) \quad \text{Eq. 5.1}$$

$$Y_{i,upper} = f(x_{i,max}, x_{\sim i,base}) \quad \text{Eq. 5.2}$$

$$Y_{i,lower} = f(x_{i,min}, x_{\sim i,base}) \quad \text{Eq. 5.3}$$

Percentage change in model outputs with respect to the base case is then calculated as follows:

$$P_{i,upper} = 100 \times \frac{Y_{i,upper} - Y_{base}}{Y_{base}} \quad \text{Eq. 5.4}$$

$$P_{i,lower} = 100 \times \frac{Y_{i,lower} - Y_{base}}{Y_{base}} \quad \text{Eq. 5.5}$$

5.2.3 Global Sensitivity Analysis

As for the model parameter sensitivity analysis, Sobol's method (2001) is selected for GSA, as it enables the impacts of interactions between specific control handles pairs, as well as those of individual control handles and higher order interactions, on key model outputs to be distinguished. It is more effective at identifying interactions between variables in highly non-linear models than alternatives such as analysis of variance, gives a more detailed description of the effects of individual control handles and their interactions, and provides more robust sensitivity rankings (Tang et al. 2007b). Further detail on Sobol's method is given in Section 4.3.2.

In this study, first and total order indices are calculated for each individual control handle and second order indices for each control handle pair. Total order indices (S_{Ti}) represent the percentage contribution of control handle i to output variance, taking into account the effects of interactions of all orders. Second order indices (S_{ij}) represent the contribution of interaction between control handles i and j only, and first order indices (S_i) the effects of control handles i alone. A high total order sensitivity index, therefore, indicates a control handle whose adjustment can affect model outputs significantly, and if the corresponding first order index is low, the contribution to output variance is predominantly due to interaction effects.

Sobol's method is implemented as detailed in Section 4.3.2, with first, second and total order sensitivity indices and corresponding 95% bootstrap confidence intervals calculated for each control handle or control handle pair.

GSA included all control handles detailed in Table 5.1, as all except two were found to have significant effects in OAT sensitivity analysis and the impact of interactions involving these is unknown. Analysis used a sample size of 2,000, which yielded 30,000 control handle sets for simulation when resampled. This value was selected on the basis of previous studies, in which it was found sufficient to achieve accurate and repeatable results with 18 and 21 parameters (Tang et al. 2007a, Fu et al. 2012). Bootstrapped confidence intervals were calculated using 1,000 resamples.

5.3 Simulation Strategy and Performance Assessment

The importance of developing GHG emission mitigation strategies based on dynamic simulations has been highlighted previously (Corominas et al. 2012, Guo et al. 2012b), and significant differences in N₂O emissions modelled under steady-state and dynamic conditions have been identified (Guo et al. 2012b). Sensitivity analysis, therefore, uses dynamic simulations to calculate key performance indicators. Simulations for assessment of control strategy performance in the BSM2 use 200 days of constant influent to allow the model to reach steady state, followed by 609 days of dynamic influent (of which the final 364 are for evaluation) (Jeppsson et al. 2007). This strategy is replicated for OAT sensitivity analysis of control handles in BSM2-e, with the model used in its open loop configuration (i.e. no sensors or controllers are implemented). Given the high computational demand of such simulations (due in part to the additional complexity of modelling dynamic GHG emissions) and the large number of model evaluations required for GSA, however, it is impractical to use the full stabilisation and evaluation period for further analysis.

In order to identify suitable reduced stabilisation and evaluation periods, additional OAT sensitivity analyses were undertaken and the effects of a range of different options on control handle rankings analysed. Maintaining a sufficiently long stabilisation period to reach dynamic 'pseudo steady state' was prioritised over the evaluation duration; given that the default SRT of the anaerobic digester is 19 days, the model may not reach quasi steady-state with

a reduced stabilisation period, but the stabilisation must be sufficient to allow the relative significance of the effects of each control handle to be assessed. Based on the OAT sensitivity analysis results, it was decided to use a 200 day steady-state simulation (using the BSM2 constant influent data but with temperature adjusted to equal that at the start of the dynamic influent) followed by a 56 day dynamic simulation (using days 294-350 of the BSM2 dynamic influent data), with the final 14 days used for performance evaluation. Although not fully replicating model outputs from the full length simulation (since the model may not reach quasi steady state with the reduced period of dynamic influent preceding the evaluation, and performance will differ throughout the year), this reduced period was found to be suitable for assessing the relative importance of each control handle: it allowed correct identification of the most sensitive control handles and resulted in a mean absolute change in OAT sensitivity analysis rank of just 0.71 for all control handles across the three key outputs when compared with the results of analysis using the full, 609 day dynamic simulation period.

Use of a shortened evaluation period provides additional benefits: if change in a specific control handle can have opposite effects depending on the state of the system (e.g. due to interaction with temperature), the resultant variance in mean performance over an extended period may be small, despite the control handle potentially being of importance. Such control handles are less likely to be overlooked with a short evaluation period and are of great interest since their dynamic control could be particularly advantageous. For sensitive control handles it is still important that potentially differing effects throughout the year are considered in control strategy development, however, since assumption that their behaviour remains as reported in this study could lead to process control related problems.

Average total GHG emissions per unit of wastewater treated are calculated to enable identification of control handles with the greatest overall effects on GHG emissions. Emissions of each individual gas from each individual source are also calculated, to allow more in-depth investigation into the greatest sources of variability and identification of critical sources. Emissions are expressed in units CO₂e to take into account the differing effects of each GHG on global warming

and enable the relative significance of emissions from different sources to be assessed.

Given that design of a WWTP control strategy must also ensure that an acceptable effluent quality is achieved at a reasonable cost, performance is assessed using EQI and OCI, as defined by Jeppsson *et al.* (2007) and detailed in Sections 3.6.2 and 3.6.3 respectively.

5.4 Results and Discussion

5.4.1 Impacts of Adjusting Operational Parameters Individually

The results of OAT sensitivity analysis of the control handles with respect to EQI, OCI and total GHG emissions are presented in Tornado diagrams (Figure 5.2). The percentage changes in each model output with respect to the base case, resulting from adjustment of each control handle to its upper and lower bounds individually, are shown and effects of increasing and decreasing control handle values are distinguished.

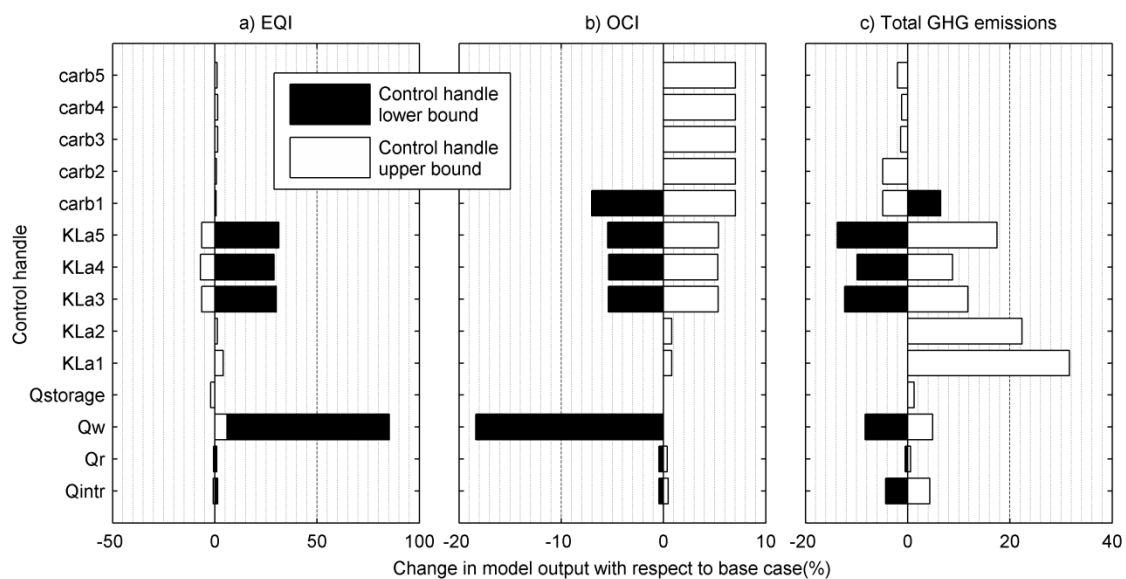


Figure 5.2: Percentage change in model outputs resulting from individual variation of control handles

It is shown that considering the effects on GHG emissions when developing control strategies to improve effluent quality and/or reduce cost is vital, since trade-offs are identifiable and, in some instances (such as *KLa1* and *KLa2*), small changes in EQI and/or OCI resulting from the first order effects of

adjusting a control handle correspond with a significant change in GHG emissions.

OAT sensitivity analysis suggests that GHG emissions are affected predominantly by aeration intensities and that increasing aeration in any of the reactors would result in an increase in emissions with respect to the base case. On average, 101% of this observed increase in net total GHG emissions is attributed to increases in direct N_2O emissions: this is as expected since high DO concentrations due to over aeration contribute to high N_2O emissions during denitrification (Kampschreur et al. 2009) and N_2O has a high GWP. Reducing aeration intensities KLa_3 , KLa_4 , and KLa_5 significantly reduces GHG emissions; however, there is a trade-off between performance indicators, and EQI is increased by over 35%.

The greatest change in total GHG emissions (32%) is achieved when KLa_1 is set to its upper bound. This knowledge may not enable development of improved control strategies, since adjustment of KLa_1 is shown only to worsen all three key performance indicators, but the fact that adjustment of KLa_1 has such a significant impact on GHG emissions compared with that on EQI and OCI highlights the importance of selecting suitable aeration intensities when developing control strategies. It may not be reasonable to actually operate the WWTP with control handles at the values tested, as satisfactory effluent quality would not be achieved – for example, KLa_1 is typically set to zero since the first reactor is anoxic, but an increase would introduce aerobic conditions and severely reduce the denitrification capacity of the plant. Decreasing aeration rates in the aerobic reactors to reduce emissions could also substantially increase the EQI. The relative significance of each control handle in terms of each model output may differ when varied only within a range that provides an acceptable level of treatment. However, trade-offs must be considered and in some cases, although undesirable, it may be that a deliberate reduction in nitrogen removal is a possible means of reducing emissions in an affordable manner.

EQI and OCI are affected most significantly by Q_w : reducing Q_w to its lower bound (giving a SRT of 46 days, within the range of an extended aeration system) results in an 85% increase in EQI and an 18% reduction in OCI. It is only ranked 6th based on its impact on GHG emissions, but a decrease in

emissions corresponds with a decrease in OCl, suggesting that the most cost effective choice of flow rate to achieve the required effluent quality will also perform favourably in terms of GHG emissions. Change in energy consumption associated with pumping provides negligible (<0.2%) contribution to the observed net change in emissions resulting from decreased Q_w , whilst direct emissions from activated sludge and the digester contribute 58% and 32% respectively. It is not, however, proposed that Q_w be decreased to the extent modelled here, due to the significant adverse effects on effluent quality.

Adjustment of carbon source addition rates may offer potential for reducing GHG emissions, based only on their individual effects – it is known that a low COD/N ratio can increase N_2O emissions from denitrification (Shahabadi et al. 2009), and it is found that increasing *carb1* or *carb2* to their upper bound value results in a 4.9% reduction in GHG emissions with negligible (up to 0.8%) trade-off in EQI. This is, however, at the expense of OCl, which increases by 7.0% (predominantly due to costs of providing the additional carbon). No single control handle can be adjusted to improve all three performance indicators simultaneously, reinforcing the importance of considering interaction effects in control strategy development and suggesting that trade-offs may be necessary.

5.4.2 Relative Significance of First, Second and Total Order Effects of Operational Parameters

Control handles are classified as ‘highly sensitive’, ‘sensitive’ or ‘non-influential’ based on their first, second and total order contributions to output variance: a sensitivity index greater than 0.1 (i.e. a contribution of at least 10%) denotes a highly sensitive control handle and a sensitivity index greater than 0.05 (i.e. a contribution of at least 5%) a sensitive control handle. Any small discrepancies observed between first/second/total order indices are fully resolved if confidence intervals are considered.

For clarity, confidence intervals are only presented for first and total order indices greater than 0.05. It is noted that some confidence intervals are large, however, the impact on control handle classification is small: all control handles classed as highly sensitive based on any of the key model outputs retain at least a sensitive classification if lower confidence bounds are used. No key control handles could have been overlooked due to uncertainty in the sensitivity

indices, since no control handles currently classed as non-influential have an upper confidence bound above the highly sensitive limit.

Some slightly negative indices are observed for all performance indicators; these are assumed to equal zero, as in previous studies (Tang et al. 2007a, Tang et al. 2007b), since it is known that truncation of Monte Carlo approximations used to calculate integrals in Sobol's method can lead to small numerical errors (Tang et al. 2007b). This also accounts for instances in which the total order sensitivity index is less than the sum of the first and second order indices (which are observed primarily for non-influential control handles), and the fact that first order indices based on OCI sum to 1.03.

First and Total Order Sensitivity Indices

Total order sensitivity indices calculated based on EQI, OCI and total GHG emissions are presented in Figure 5.3, with the contribution of first and higher order effects shown.

In terms of their total order effects on GHG emissions, three control handles are classified as highly sensitive: Q_w , $KLa1$ and $KLa5$. Q_w is also the greatest contributor to output variance in EQI and OCI and appropriate control of this control handle is, therefore, vital. The importance of wastage flow rate in terms of its effects on effluent quality and operational costs is already recognised, but by showing the sensitivity of GHG emissions to this control handle, this study highlights the necessity to consider all three performance indicators when selecting an appropriate value. EQI and OCI are also both either sensitive or highly sensitive to variation in $KLa5$, suggesting that selection of an appropriate aeration intensity is key to the reduction of GHG emissions whilst maintaining an acceptable effluent quality and cost. This appears intuitive, since energy requirements for pumping and aeration contribute to both costs and emissions, yet it has been established in OAT sensitivity analysis that these control handles have a much greater effect on direct emissions than on those associated with energy consumption.

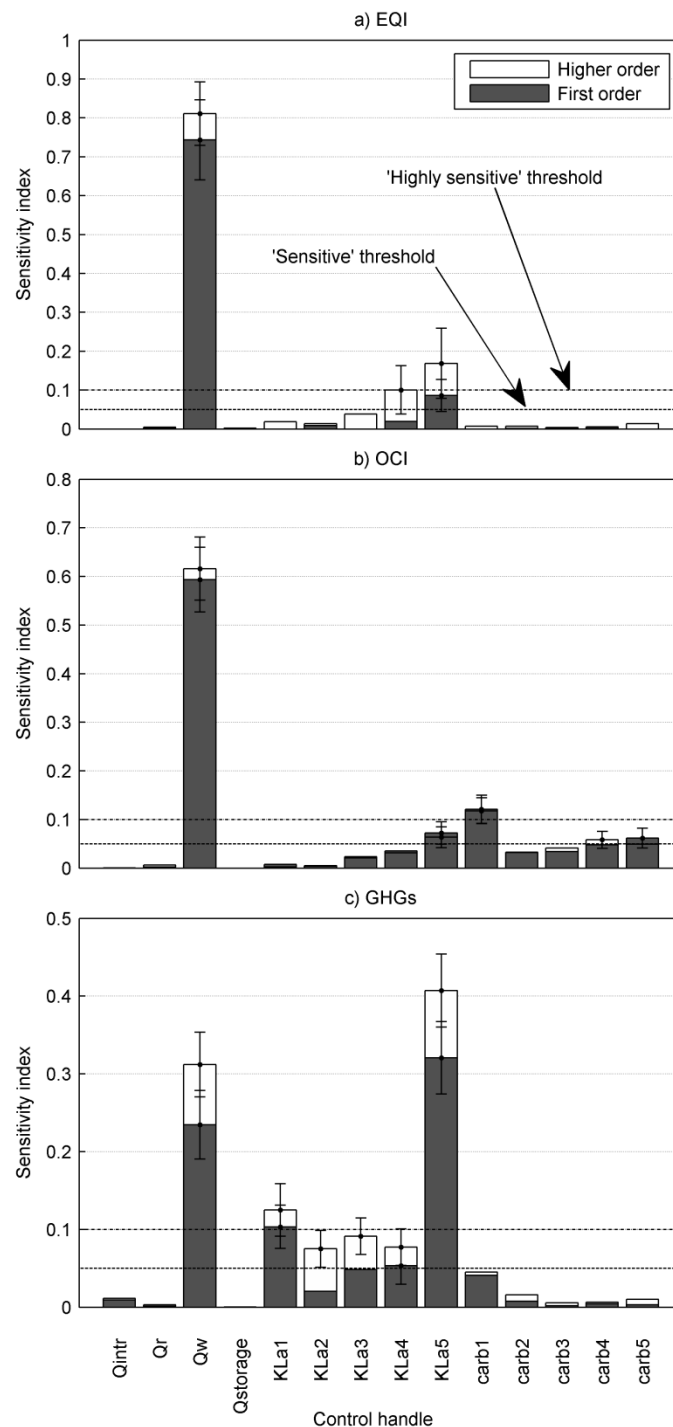


Figure 5.3: First and total order indices calculated using Sobol's method, based on EQI, OCI and total GHG emissions

The aeration intensities *KLa1-4* all have a significant impact on GHG emissions but provide a greater contribution to output variance in emissions than in EQI, suggesting that a reduction in emissions with comparatively little impact on effluent quality should be achievable. Furthermore, reducing emissions without incurring additional costs may be possible since all control handles to which

GHG emissions are sensitive, except Q_w , have a higher total order sensitivity index based on GHG emissions than on OCI.

It is also found that interactions between control handles have a significant impact on both GHG emissions and EQI, accounting for 15% of variance in each output. As such, effective design of control strategies to reduce GHG emissions will need to consider the effects of using multiple control handles simultaneously and may require complex control algorithms. Model predictive control of the DO setpoint and external carbon flow rate, for example, has been shown to enable reduced operating costs and improved effluent quality (Stare et al. 2007), although GHG emissions have not been considered.

GSA results show that neither EQI, OCI nor GHG emissions are sensitive to adjustment of Q_{intr} , Q_r , $Q_{storage}$, $carb2$ or $carb3$ values (within the tested ranges), so optimisation of their values is of low priority and can be omitted to simplify the design problem. Note, however, that the sensitivity classification will be affected by the range considered for each control handle and if a disproportionately narrow range is used then the sensitivity indices will be lower than expected. This is relevant particularly in the case of return sludge flow rate (Q_r), which is classified as non-influential here but could in reality take values outside the range considered and therefore have greater influence. Aeration intensities used may also be lower than suggested if the nitrogen load to the plant is reduced. However, whilst this may change the relative importance of these control handles, it would only increase their influence. Given that they are already classified as sensitive or highly sensitive, it would not alter the conclusions of this study. If necessary, further research could be undertaken to investigate the sensitivity of control handle classification to the choice of upper and lower bounds.

Reduction of OCI – or correlation of OCI with chosen control handle values – ought to be straightforward since GSA reveals no significant interaction effects and shows variance to be predominantly (62%) attributable to variation in Q_w .

Second Order Sensitivity Indices

Second order indices are presented in Figure 5.4, in which the darkest colours denote control handle pairs to which the corresponding output is most sensitive. Control handle pairs individually accounting for more than 5% are identified and,

whilst no specific pairs are classified as sensitive based on more than one model output, all sensitive pairs (for any model output) are found to include *KLa5*. This reinforces the importance of controlling *KLa5* if GHG emissions are to be reduced and an acceptable effluent quality maintained, and shows that interactions of *KLa5* with *Qw*, *KLa3*, *KLa4*, *carb1*, *carb2* and *carb3* must be taken into account. This appears reasonable since it is known, for example, that a low SRT, insufficient COD availability and low DO concentrations can lead to nitrite accumulation, which in turn can contribute to high N₂O emissions (Kampschreur et al. 2009). It must be noted, however, that the impacts of *KLa5* adjustments and interactions may differ in practice due to model limitations; in this study, changes in *KLa5* have a large impact on conditions in the first reactor due to the use of a standard non-reactive clarifier model, but creation of anoxic conditions due to oxygen consumption can occur in a reactive clarifier (Guerrero et al. 2013), thereby preventing or reducing recirculation of oxygen.

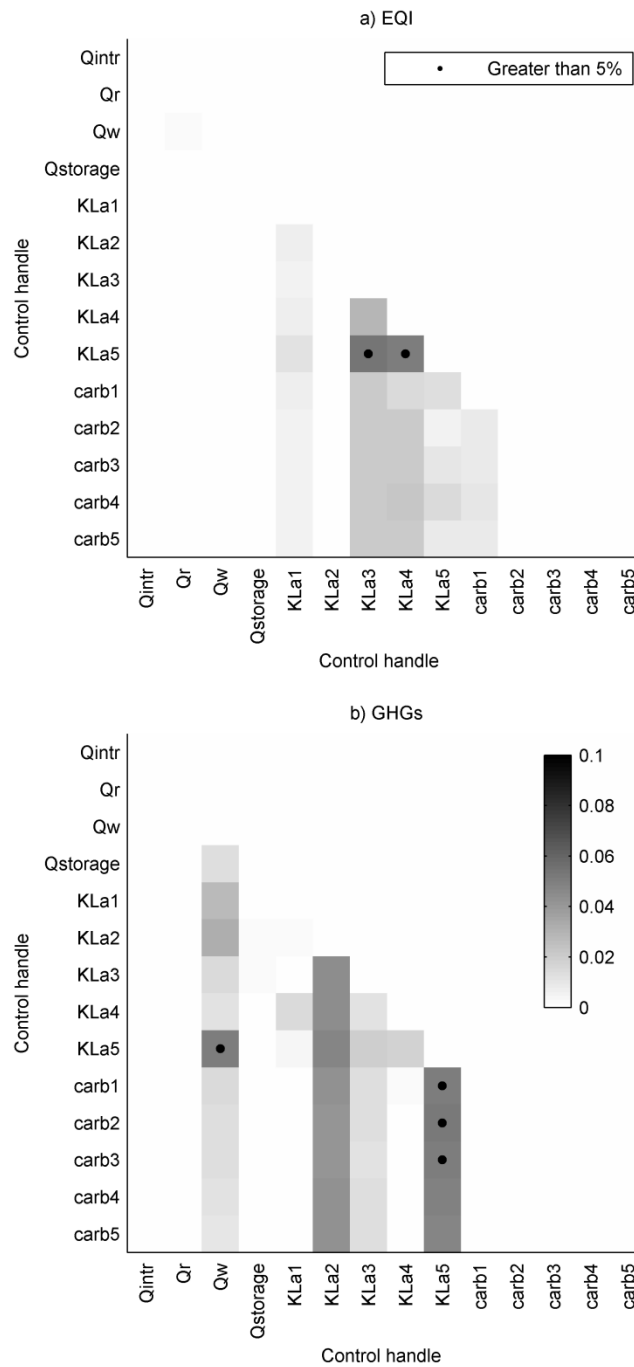


Figure 5.4: Second order sensitivity indices calculated using Sobol's method based on EQI and total GHG emissions

For the EQI, no significant second order effects involving Qw are identified, showing that interaction effects visible in Figure 5.4 must be due to higher order effects. Selection of appropriate control handle values to improve effluent quality will be challenging, therefore, since Qw is the greatest source of output variance and must interact with multiple control handles.

Analysis of the first and total order indices shows interaction effects to have negligible impact on the OCI, with only Qw involved in any identifiable interactions. This corresponds with the second order indices, in which no sensitive control handle pairs are found and the only interactions of note involve Qw.

5.4.3 Key Control Handles for Control Strategy Design to Reduce Greenhouse Gas Emissions

The results of OAT sensitivity analysis are used in conjunction with those of GSA to identify key control handles for the design of control strategies to reduce GHG emissions, since they give an indication of the likely direction of change whilst GSA explores the whole control handle space. To enable comparison, control handle rankings derived from the two analyses are summarized in Table 5.2. Results are also compared to identify important control handles which may be overlooked based on OAT sensitivity analysis alone. Control handles found to be most important in OAT sensitivity analysis are found to have significant effects in GSA, confirming that sensitive control handles have not been overlooked due to the reduced model stabilization and evaluation periods.

Table 5.2: Ranking of control handles based on OAT sensitivity analysis and GSA

	Sensitivities based on EQI			Sensitivities based on OCI			Sensitivities based on total GHG emissions		
Control handle	GSA sensitivity		OAT rank	GSA sensitivity		OAT rank	GSA sensitivity		OAT rank
	rank			rank			rank		
	First order	Total order		First order	Total order		First order	Total order	
Qintr	10	13	6	13	13	13	8	9	8
Qr	8	11	8	12	10	10	12	13	12
Qw	1	1	1	1	1	1	2	2	6
Qstorage	6	14	7	14	14	14	14	14	14
KLa1	14	5	5	10	12	11	3	3	1
KLa2	4	6	11	11	11	13	7	6	4
KLa3	12	4	3	9	9	4	5	4	3
KLa4	3	3	4	6	8	5	4	5	5
KLa5	2	2	2	3	3	3	1	1	2
carb1	13	8	14	2	2	2	6	7	7
carb2	7	9	13	8	7	7	9	8	9
carb3	9	12	10	7	6	6	13	12	13
carb4	5	10	9	5	4	6	10	11	13
carb5	11	7	12	4	5	8	11	10	10

Light grey shading denotes sensitive control handles, based on corresponding index

Dark grey shading denotes highly sensitive control handles, based on corresponding index

OAT sensitivity analysis correctly identifies control handles classified as highly sensitive based on EQI and OCI in GSA as having the most significant effects. However, it does not enable identification of all control handles to which GHG emissions are highly sensitive due to the greater significance of interaction effects: Qw is ranked only 6th in OAT sensitivity analysis, but GSA shows it to be the second most important control handles, with its interactions contributing 7.7% of output variance. Simultaneous manipulation of Qw (to adjust SRT) and other control handles (such as aeration intensities) is an established approach to WWTP control, and the potential for improvements in effluent quality and operational costs has been demonstrated (e.g. Guerrero et al. 2012), but these results highlight the importance of considering interaction effects on GHG emissions also. No control handles which enable simultaneous improvement in

EQI, OCI and GHG emissions through their first order effects alone were found, but trade-offs may be lessened or avoided when interactions are considered.

In this study, the impact of Q_w on EQI is shown to be predominantly due to first order effects and OAT sensitivity analysis results suggest that adjustment is only likely to worsen effluent quality. It is also shown, however, that GHG emissions and OCI can both be reduced through the first order effects of Q_w . Given that interaction effects with Q_w do contribute to variance in EQI, and significantly to variance in GHG emissions, simultaneous improvements which are not revealed through OAT sensitivity analysis alone might be possible through appropriate control of Q_w and its interacting control handles.

All three outputs are sensitive or highly sensitive to adjustment of KLa_5 . However, OAT sensitivity analysis shows that a decrease in KLa_5 corresponds with a significant reduction in GHG emissions and OCI but an increase in EQI, so adjustment to reduce emissions whilst maintaining acceptable effluent may not be straightforward. An increase in KLa_5 results in a small improvement in EQI but significantly worsens GHG emissions; this reinforces the necessity to consider the effects on GHG emissions when control is modified to improve effluent quality and supports previous recommendation that GHG emissions should be included as an evaluation criterion to provide a clearer picture of the overall suitability of WWTP control strategies (e.g. Flores-Alsina et al. 2014). GSA also shows KLa_5 to be involved in significant interaction effects, further complicating the design problem. In particular, the effects of interaction with Q_w on GHG emissions and interaction with KLa_3 on EQI should be considered.

GHG emissions are found to be highly sensitive to KLa_1 and sensitive to KLa_2 , whilst effects of these control handles on EQI and OCI are insignificant. This might imply that adjustment of KLa_1 and KLa_2 could be used to reduce emissions without incurring trade-offs; however, the base case value for both is zero and OAT sensitivity analysis shows only a significant increase in emissions resulting from change in KLa_1 and KLa_2 . Therefore, although they have a significant impact on GHG emissions, there may be no benefits from altering the base case values as performance would only be worsened. Given the high sensitivity of KLa_1 , however, it is recommended that the effects of small alterations are investigated since these would be missed in OAT sensitivity analysis and may be beneficial.

Interaction effects involving *KLa3* are shown to be particularly important, as GHG emissions would not be classified as sensitive to this control handle based on its first order effects alone. Given that neither EQI nor OCI are sensitive to *KLa3* and OAT sensitivity analysis shows that adjustment to reduce emissions is possible, suitable control of aeration in the first aerobic reactor is likely to be key to the development of control strategies to reduce GHG emissions – although complex, given interactions mostly involve at least three control handles.

Appropriate control of *KLa4* is also important, since it is classified as sensitive based on both EQI and GHG emissions. OAT sensitivity analysis reveals a trade-off: a reduction in GHG emissions due to individual adjustment of *KLa4* corresponds to an increase in EQI, but because GSA shows the effects of interactions to involving *KLa4* to be significant, it is likely that the comparative magnitude of effects on each output differs across the range of feasible values and an optimum can be identified.

In GSA, *carb1* is classified as sensitive based on OCI only and, as such, might be adjusted in an attempt to reduce cost with little impact on effluent quality or emissions. However, OAT sensitivity analysis shows that a decrease in OCI due to reduction of *carb1* corresponds with an increase in GHG emissions. Therefore, if *carb1* is lowered to reduce operational cost, it is vital that the impact on GHG emissions is considered and, if necessary, countered with other measures.

EQI, OCI and GHG emissions are not sensitive to *Qintr*, *Qr*, *Qstorage*, *carb2* and *carb3* within the tested ranges, suggesting that dynamic control of these control handles would be of little benefit. It is, therefore, recommended that optimisation of internal recirculation flow rate, return sludge flow rate, anoxic reactor carbon source addition rates (except in first reactor) and storage tank control is of low priority when developing new WWTP control strategies. It has been demonstrated that control strategy optimisation using this knowledge can enable substantial emission reductions whilst maintain an acceptable effluent quality and without increasing operational costs (Sweetapple et al. 2014b).

5.4.4 Key Emission Sources for the Reduction of Greenhouse Gas Emissions

Based on simulations undertaken for GSA, the base case value, mean and variance of emissions from different sources are detailed in Table 5.3. Total GHG emissions are decomposed into direct emissions of each gas and indirect emissions from each source, as well as those resulting from the wastewater line and sludge line. Wastewater line emissions include all direct emissions associated with the activated sludge reactors and indirect emissions resulting from effluent degradation and energy demand for reactor aeration and mixing, chemical consumption; sludge line emissions include those from biogas leakage, combustion and energy recovery, dewatering, energy for digester heating and mixing, and transport and offsite degradation of sludge. It is noted that variances reported are small in comparison with those resulting from model parameter uncertainties (Sweetapple et al. 2013), and future work should investigate the impact of modelling uncertainties on control strategy design.

Table 5.3: Characteristics of GHG emissions from key sources

	Direct emissions				Indirect emissions			Total wastewater line	Total sludge line	Total GHGs
	Direct CO ₂	Direct CH ₄	Direct N ₂ O	Net energy	Carbon source	Reactor effluent offsite GHGs	Sludge offsite GHGs			
Base case (kg CO ₂ e/m ³)	0.47	0.06	0.15	0.06	0.04	0.03	0.06	0.55	0.32	0.87
Mean (kg CO ₂ e/m ³)	0.47	0.06	0.24	0.06	0.06	0.03	0.05	0.66	0.32	0.98
Variance ((kg CO ₂ e/m ³) ²)	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.02	0.00	0.03

It is notable that, whilst direct CO₂ emissions are the greatest contributor to mean total GHG emissions (at 48%), their output variance is just 1.7% of that of direct N₂O emissions, which contribute only a comparatively small 24% of mean total GHG emissions. Indirect emissions and direct CH₄ emissions contribute 28%, yet are found to have negligible variance. This shows that the source of emissions with the greatest scope for improvement does not necessarily correspond with the overall greatest source of emissions, and suggests that any reduction in GHG emissions resulting from modified control will be primarily due to a reduction in N₂O emissions. Control strategy development and optimisation

should, therefore, focus on reduction of direct N₂O emissions, all of which result from wastewater processes (specifically, activated sludge), and it is important that N₂O emissions are carefully monitored to ensure that they are not unintentionally increased as a result of actions to improve effluent quality and/or reduce operational costs. Existing knowledge that a reduction in DO setpoint to reduce costs can result in an increased risk of N₂O production (Porro et al. 2014) supports this recommendation. A potential strategy for mitigating the risk whilst maintaining cost savings may include better control and distribution of the aeration (Porro et al. 2014).

Further sensitivity analysis is used to investigate key control handles affecting wastewater line and sludge line GHG emissions, and OAT sensitivity analysis results are presented in Figure 5.5 (calculations provided in Appendix A).

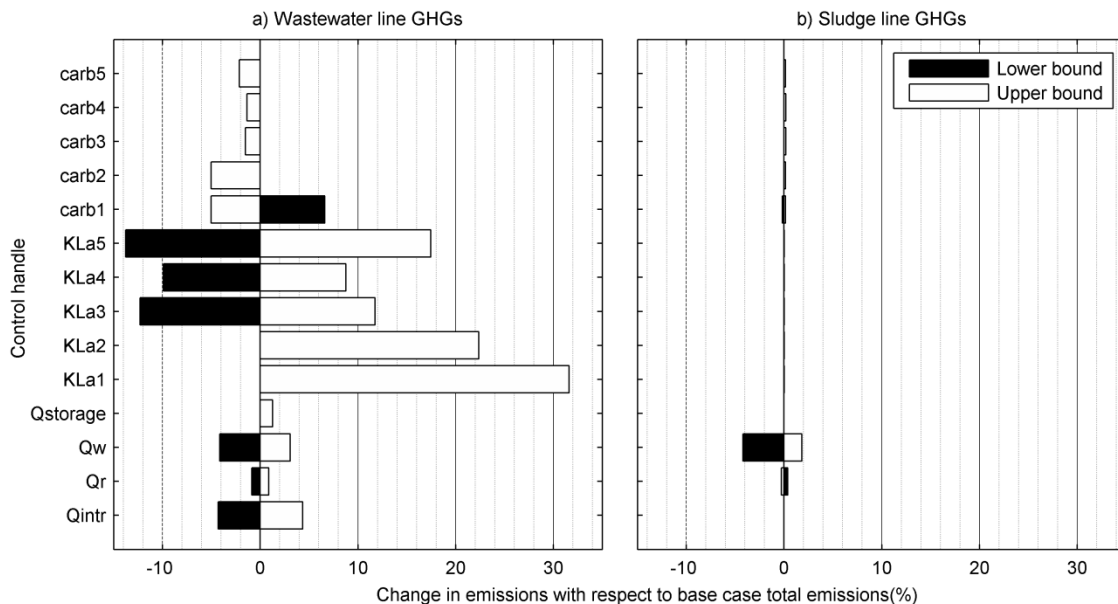


Figure 5.5: Change in wastewater line and sludge line GHG emissions resulting from variation of individual control handles, as a percentage of base case total GHG emissions

In OAT sensitivity analysis it is shown that changes in total GHG emissions are predominantly due to variation in wastewater line emissions, with only Qw resulting in a change of emissions of more than 0.7% in the sludge line. In GSA also, variance in sludge line emissions is negligible in comparison with that of wastewater line emissions and is found to be primarily due to the first order effects of Qw. The ranking of each control handle based on total order effects on wastewater line emissions is identical to that for total GHG emissions, but an

additional sensitive control handle, *carb1*, is identified. The significance of first order effects of variation in *KLa3* is also greater on wastewater line emissions than on total emissions, with the control handle now classified as sensitive based on its first order index.

OAT sensitivity analysis shows a decrease in Q_w , the only control handle to which sludge line emissions are sensitive, to correspond with a decrease in both sludge line and wastewater line emissions (and vice versa). WWTP modelling used during control strategy development for the reduction of GHG emissions could, therefore, justifiably omit sludge line emissions in order to reduce computational demand, since there is little potential for their reduction from improved control alone and any small change observed is likely to be a decrease if Q_w is manipulated to aid reduction of wastewater line emissions.

5.5 Conclusions

This research has investigated the impact of adjusting 14 WWTP control handles, including flow rates, aeration rates and carbon source addition rates, to enable identification of key control handles and sensitive sources for the reduction of GHG emissions. Based on the results of OAT sensitivity analysis and Sobol's method GSA, the following conclusions are drawn:

- It is vital to consider the effect on GHG emissions when developing control strategies to improve effluent quality and/or reduce cost as, in some instances, a small change in EQI and/or OCI resulting from the individual effects of adjusting a control handle corresponds with a significant change in GHG emissions, and trade-offs between objectives have been identified.
- Selection of suitable values for aeration intensity in the final tank and wastage flow rate in the activated sludge process is of key importance, and active control of these control handles may be beneficial, but it is essential that their impacts on GHG emissions are considered. Both have a significant individual impact on variance in all three model outputs, and EQI and GHG emissions are also sensitive to interaction effects involving the aeration intensity.
- Unless effluent quality and/or operational cost are to be sacrificed, it is necessary to consider the effects of adjusting two or more control

handles together when developing control strategies to reduce GHG emissions, since no control handles enabling simultaneous improvement in EQI, OCI and GHG emissions through their individual effects alone were identified.

- Formation of N_2O in the activated sludge process is the source of GHG emissions with the greatest scope for improvement, and from which it is important that emissions are carefully monitored to ensure that they are not unintentionally increased as a result of actions to improve effluent quality and/or reduce operational costs.

This knowledge will assist development of WWTP control strategies to reduce GHG emissions whilst maintaining acceptable effluent quality and operating costs, and aid an efficient design and optimisation process.

6 WASTEWATER TREATMENT PLANT CONTROL STRATEGY DEVELOPMENT AND OPTIMISATION

6.1 Multi-Objective Optimisation of Wastewater Treatment Plant Control to Reduce Greenhouse Gas Emissions

Appropriate WWTP operation can contribute greatly to the reduction of GHG emissions (Gori et al. 2011) and it has been shown that implementing automatic control in WWTPs can have a significant impact on GHG emissions, with reductions of up to 9.6% achieved by Flores-Alsina et al. (2011). However, the existence of trade-offs and the need for a balancing act has been highlighted (Flores-Alsina et al. 2011), and a thorough investigation into the relationships and trade-offs between GHG emissions, effluent quality and operational costs is needed to enable assessment of the potential improvements achievable in existing WWTPs by altering only the control of the system. Multi-objective optimisation enables the identification of a set of Pareto-optimal solutions, which are non-dominated based upon a given objective set (i.e. cannot be further improved in terms of any one objective without worsening another); this solution set can be used to illustrate trade-offs between objectives.

The effects of implementing a range of different control strategies and of using different setpoints for control on GHG emissions, effluent quality and operational costs have been explored previously (Flores-Alsina et al. 2011, Guo et al. 2012b). Based on this, recommendations regarding the control of WWTPs to provide high quality effluent with low operational GHG emissions have been made (e.g. Flores-Alsina et al. 2011, Guo et al. 2012a, Guo et al. 2012b, Flores-Alsina et al. 2014). The importance of using multiple objectives to evaluate and compare WWTP control strategies has been highlighted previously (Flores-Alsina et al. 2014), and trade-offs between effluent quality and operational costs have been identified using multi-objective genetic algorithms for the optimisation of controller setpoints (Beraud et al. 2007, Tomita and Park 2009). However, conclusions drawn from previous studies regarding the reduction of GHG emissions are based on WWTP performance under only a limited number of different control scenarios, and a global, multi-objective optimisation of multiple operational parameters has not been used to investigate further improvements achievable or the existence of additional optimal solutions.

This section of the thesis, therefore, aims to investigate the potential of control strategy optimisation for the reduction of operational GHG emissions resulting from wastewater treatment, and to investigate necessary trade-offs between conflicting control objectives. This is achieved by multi-objective optimisation of the control of an activated sludge WWTP, in which aeration intensities are manipulated in order to maintain a specified DO concentration. Objectives considered include the minimisation of GHG emissions, operational costs and effluent pollutant concentrations whilst maintaining legislative compliance. The intention of this research is not to prescribe a specific control strategy that can be used to reduce emissions, since the model used is of a hypothetical plant and there are (necessarily) omissions in the sources of GHG emissions modelled, rather to demonstrate that – assuming the model represents the real phenomena reasonably well – improvements can be realised if optimised control strategies from multi-objective optimisation are implemented.

6.1.1 Wastewater Treatment Plant Model

Model Scope

The modelled WWTP is based on BSM2-e. BSM2-e is computationally demanding, however, and unsuitable for multi-objective optimisation given the high simulation time and large number of simulations required. Reductions in GHG emissions resulting from improved plant control have been previously attributed predominantly to differences in power consumption and secondary treatment process emissions (Flores-Alsina et al. 2011), and sensitivity analysis (Chapter 5) has found there to be negligible variance in sludge line emissions resulting from adjustment of operational parameters (Sweetapple et al. 2014a). This suggests that the most significant improvements in total GHG emissions resulting from control strategy optimisation will be due to a reduction in emissions resulting from wastewater rather than sludge treatment processes and that modelling of the wastewater treatment processes alone is sufficient to demonstrate the potential of control strategy optimisation to reduce GHG emissions. The BSM2-e model is, therefore, modified to exclude sludge treatment, significantly reducing simulation time and thereby making multi-objective optimisation feasible. Modelling of all operational parameters to which effluent quality, operational cost or GHG emissions are sensitive is retained (Sweetapple et al. 2014a).

The layout of the reduced model is shown in Figure 6.1 and consists of a primary clarifier, an activated sludge reactor containing two tanks which may be operated under anoxic or aerobic conditions, followed by three aerobic tanks in series, a secondary settler and a sludge thickener. The primary clarifier has a volume of 900m^3 , assumes a 50% solids removal efficiency and is modelled based upon Otterpohl (1995). The anoxic tanks have a volume of 1500m^3 each and the aerobic tanks volumes of 3000m^3 each; both are modelled using a version of the ASM1 (Henze et al. 2000) modified for inclusion of GHG emissions as detailed in Chapter 3 and by Sweetapple et al. (2013). The secondary settler has a surface area of 1500m^2 , volume of 6000m^3 , and is modelled based upon Takács et al. (1991). Sludge thickening is modelled as an ideal and continuous process, with no biological activity and assuming 98% solids removal efficiency.

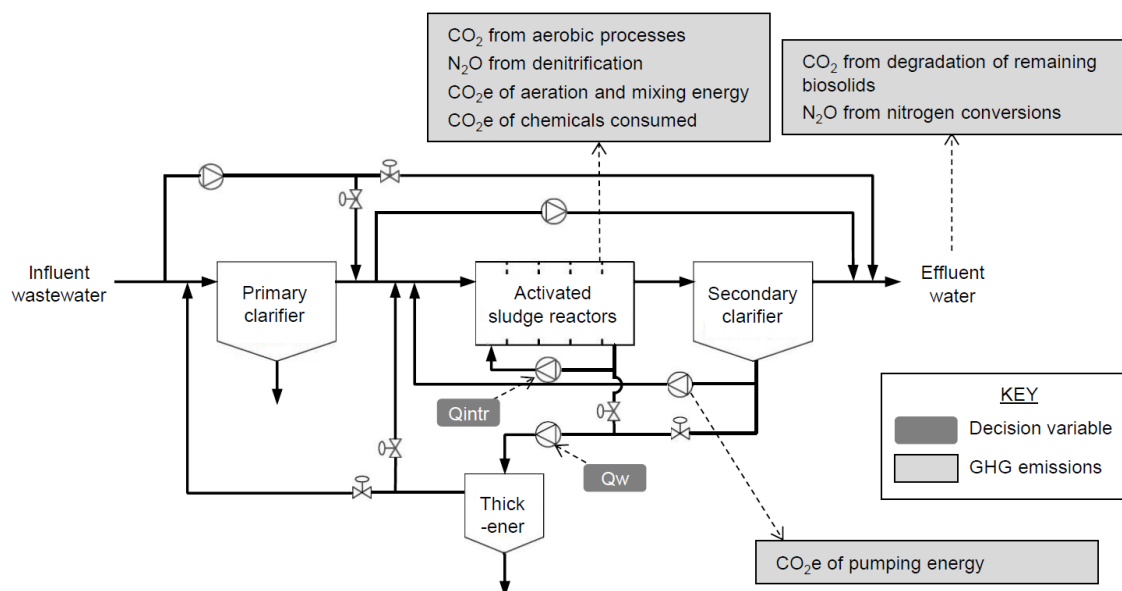


Figure 6.1: WWTP model layout and modelled sources of GHG emissions

Modelled GHG emissions include direct emissions from the activated sludge reactors and indirect emissions resulting from manufacture of chemicals, energy generation and offsite effluent degradation. Dynamic production of N_2O due to incomplete denitrification, associated CO_2 emissions, and CO_2 formed during substrate utilisation and biomass decay in the activated sludge units are modelled as in BSM2-e, as are CO_2 and N_2O emissions from aerobic degradation of the effluent. Emissions resulting from the generation of energy imported are calculated using the modelled energy requirement for activated

sludge aeration and mixing, and pumping of the internal recycle flow, return activated sludge flow, wastage flow and the primary clarifier underflow.

Control Strategy

The implementation of sensors and actuators is based on the BSM2 default closed loop control strategy, as detailed by Nopens et al. (2010) and illustrated in Figure 6.2. Key features of the control are as follows:

- A DO sensor in reactor 4
- A PI controller, with setpoint, offset, gain and integral time constant to be specified
- Manipulation of aeration intensities in reactors 3-5 (KLa_3 , KLa_4 and KLa_5)
- Controller output fed directly to KLa_4 actuator
- Input to KLa_3 and KLa_5 actuators proportional to controller output (gain for each specified separately)
- Constant aeration intensities (KLa_1 and KLa_2) in reactors 1-2.

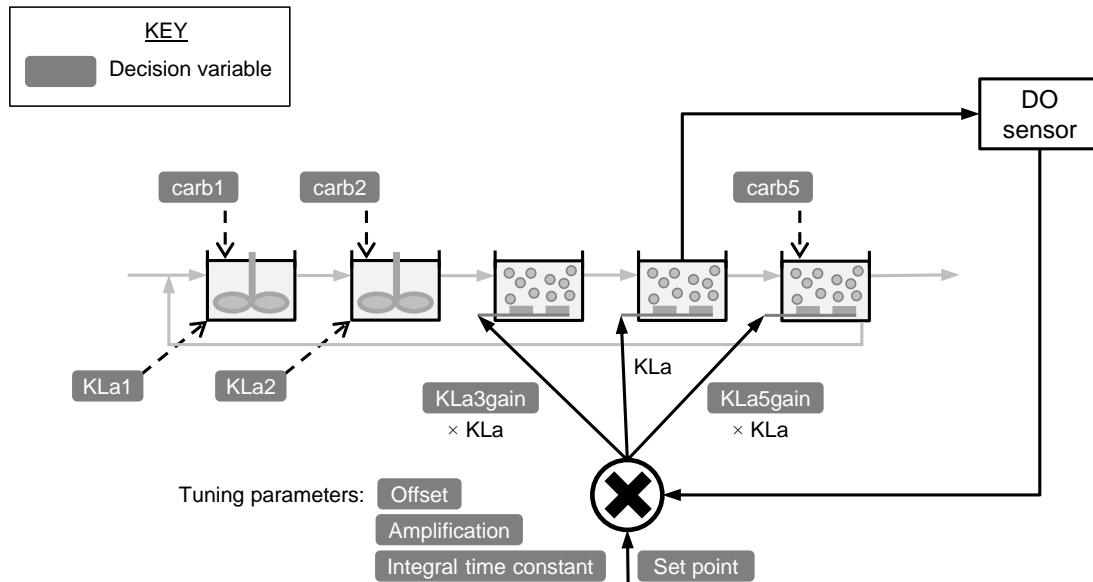


Figure 6.2: Implemented control loop, with associated decision variables identified by grey boxes

This strategy was selected since activated sludge DO control is known to affect effluent quality (e.g. Nopens et al. 2010), energy consumption / operational costs (e.g. Åmand and Carlsson 2012) and GHG emissions (e.g. Flores-Alsina

et al. 2011, Aboobakar et al. 2013). It is thought that optimisation of the control may enable further performance improvements, and KLa_3 , KLa_4 and KLa_5 have been identified as key operational parameters affecting effluent quality, operational costs and GHG emissions (Sweetapple et al. 2014a).

Sensor definitions provided in BSM2 (detailed by Alex et al. 2008) are used during control strategy development. For the purposes of testing, it is assumed that the sensor is ideal (i.e. no delay and no noise); this allows evaluation of the theoretical potential of a given control strategy. Control handle actuators have a response time of four minutes and a second order time delay function, as prescribed for KLa actuators in BSM2 (Alex et al. 2008).

The load of the activated sludge unit in this WWTP model is significantly reduced with respect to that of the BSM2, given that sludge treatment processes have been removed and there is, therefore, no reject water. The key features of the default BSM2 closed loop control strategy (a DO sensor in reactor 4 and manipulation of aeration intensities in reactors 3-5) are retained, however, since manipulation of aeration intensities using a fixed DO setpoint is practice in common in activated sludge control (e.g. Copp 2002, Belchior et al. 2012). Maintaining sufficiently high DO concentrations through the use of DO control is considered particularly important in this study given that low DO concentrations have previously been linked to high N_2O emissions (Kampschreur et al. 2009). It is recognised that the default controller parameters used in BSM2 may not perform as well in this model given the change in load, but a DO setpoint of 2 mg/l is typical when nitrification is required (e.g. Holenda et al. 2008, Rieger et al. 2012) and use of such a value is thought to provide a reasonable base case for comparison.

Simulation Strategy

Plant performance is modelled using the predefined dynamic influent data for BSM2 (Gernaey et al. 2011). Given the large number of model evaluations required for multi-objective optimisation using genetic algorithms, it is not feasible to simulate the full 609 days of dynamic BSM2 influent data for each evaluation. Additionally, a long stabilisation period was required for BSM2 due to the long-term dynamics of the anaerobic digester (Jeppsson et al. 2006), but this is not included in the modelled WWTP. Preliminary investigation has shown

that control strategy optimisation in which evaluation of plant performance is based on a single, reduced time period results in strategies which perform well during this period but poorly on average across the year, due to seasonal variations. Therefore, each control strategy is assessed over two separate 14-day periods simulated using days 245-259 and 427-441 of the BSM2 influent data, representing operation of the WWTP in summer and winter conditions respectively. Of each 14-day period, the first 7 days are for stabilisation and the last 7 for performance evaluation. Before using the dynamic data, the system is simulated under the base case closed loop control strategy using constant influent data for a 1000-day period to enable steady state to be reached; these steady state values are then used to initialise the model for each dynamic simulation.

It is recognised that an accurate measure of plant performance throughout the year cannot be obtained from only two short evaluation periods, and use of a significantly reduced dynamic stabilisation period may affect results. Further changes in model outputs may result from improved model initialisation, since the same set of steady state values is used for each simulation as it is not computationally feasible to run the steady state simulation for each of the 390,000 model evaluations undertaken. Therefore, it is recommended that the results of this study are used only to demonstrate the potential for control strategy optimisation to enable a reduction in GHG emissions and to identify performance trade-offs and trends in choice of optimum operational parameters – not to recommend a specific control strategy.

Performance Assessment

Plant performance is assessed based on average total GHG emissions per unit of wastewater treated, an EQI, an OCI, as for BSM2-e. The OCI is modified, however, to account for the removal of sludge treatment:

$$OCI = AE + PE + 3 \cdot SP + 3 \cdot EC + ME \quad \text{Eq. 6.1}$$

where:

- AE = Energy for aeration [kWh/d]
- PE = Energy for pumping the primary clarifier and thickener underflows and the activated sludge internal recirculation,

recycle and wastage flows [kWh/d]

SP = TSS accumulation in the reactors, primary clarifier and secondary settler, and TSS in the primary clarifier and thickener underflows and wastewater effluent [kg TSS/d]

EC = External carbon source addition [kg COD/d]

ME = Energy for reactor mixing [kWh/d]

Given that a low EQI does not necessarily ensure compliance with effluent quality standards, effluent quality is also assessed with regard to the UWWTD requirements. Compliance can be achieved by meeting either the minimum percentage reduction or the upper concentration limit requirements. BOD, COD and TSS compliance can still be achieved if up to 5% of samples fail to meet the required concentration, provided that the absolute maximum concentration is not exceeded on these occasions. Furthermore, extreme water quality values resulting from unusual situations such as heavy rain need not be taken into account. Total nitrogen and total phosphorus limits apply only to discharges to sensitive areas which are subject to eutrophication and the required nitrogen concentration refers to the annual average. Complete details of the UWWTD requirements are provided in Table 3.4, and those applicable to the modelled WWTP are summarised in Table 6.1.

Table 6.1: Discharge requirements for modelled WWTP under the UWWTD

Parameter	Annual 95 percentile (g/m ³)	Annual maximum (g/m ³)	Annual mean (g/m ³)
BOD ₅	25	50	-
COD	125	250	-
TSS	35	87.5	-
Total nitrogen	-	-	15

Effluent ‘ammonia and ammonium nitrogen’ is also measured as this may be consented, despite not being a specific requirement of the UWWTD. The following assumptions apply henceforth: ‘BOD₅’ refers to effluent BOD₅ 95 percentile, ‘COD’ refers to effluent COD 95 percentile, ‘TSS’ refers to effluent TSS 95 percentile, ‘nitrogen’ refers to mean effluent total nitrogen and ‘ammonia’ refers to effluent ammonia and ammonium 95 percentile.

Note that, given the modifications to the WWTP layout, results obtained in this study are not directly comparable with those from BSM2 or BSM2-e (e.g. Nopens et al. 2010, Sweetapple et al. 2013).

6.1.2 Multi-Objective Optimisation Methodology

Optimisation Algorithm

Control strategy optimisation is carried out using the Non-Dominated Sorting Genetic Algorithm-II (NSGA-II) (Deb et al. 2002), since it is computationally fast and has been shown to provide better coverage and maintain a better spread of solutions than other multi-objective evolutionary algorithms (MOEAs) (Deb et al. 2002). Local optimisation methods are very efficient in finding local optima within a convex area of the design space, but may result in suboptimal solutions for complex optimisation problems with many local optima and a highly non-linear design space. Genetic algorithms are better suited to the optimisation of WWTP control strategies due to their ability to handle nonlinearities whilst requiring fewer objective function evaluations than alternative techniques (Cosenza et al. 2009), and to find multiple optimal solutions in a single simulation run (Deb et al. 2002). Problems with multiple objectives can be tackled by transforming them into single objective problems with a weighting system applied to the objectives; in this instance, however, a MOEA is selected to enable a set of non-dominating solutions to be identified and trade-offs between objectives to be investigated without the need for a weighting system.

NSGA-II is implemented as follows:

1. Initialise the population (solution set for evaluation), $P(0)$, with random values for N individuals
2. Calculate objective values for each individual in $P(0)$
3. Fast non-domination sort of $P(0)$
4. Repeat following for t generations:
 - a. Use binary tournament selection to select parent population, $Pp(t)$, from $P(t)$
 - b. Perform crossover and mutation of $Pp(t)$ to create child population, $Pc(t)$
 - c. Form intermediate population, $Pi(t)$, from $Pp(t)$ and $Pc(t)$
 - d. Fast non-domination sort of $Pi(t)$

- e. Form next generation, $P(t+1)$ from N best individuals of $P(t)$

In the non-dominated sorting, Pareto dominance is used to rank all individuals of a population. Those which are not dominated by any other (an individual dominates another if it performs equally well in all objectives and better in at least one) are assigned a rank of 1. This procedure is repeated for the remaining population to find individuals with a rank of 2, then 3 etc.. Selection of the best solutions is based on both rank and crowding distance.

Decision Variables

Selection of operational parameters for optimisation is guided by the results of previous sensitivity analyses (Chapter 5) (Sweetapple et al. 2014a). Parameters identified as contributing significantly to variance in effluent quality, operational cost and/or GHG emissions are either included as decision variables or dynamically controlled, with the control parameters and controller tuning parameters also used as decision variables. Exceptions to this are:

- Carbon source addition rate in the fourth activated sludge reactor is not optimised despite being classed as sensitive based on OCI, since adjustment from the base case value resulted only in an increase in operational costs in one-factor-at-a-time (OAT) sensitivity analysis.
- Internal recycle flow rate (Q_{intr}) and carbon source addition rate in the second activated sludge reactor ($carb2$) are included despite not being classified as sensitive, since OAT sensitivity analysis suggests that they can be adjusted to reduce GHG emissions with negligible impact on effluent quality.

All decision variables are listed in Table 6.2, with details of their default values and range of values considered for optimisation given. Where applicable, the upper and lower bounds of control handle values are set to the default value $\pm 10\%$ of the allowable range specified in BSM2 (with the lower limit set to zero where this gives a negative number). These ranges are chosen to avoid selection of extreme, unrealistic solutions and improve the efficiency of the optimisation process. However, in some cases they are relatively narrow and it should be recognised that they do not encompass every feasible possibility. Optimised solutions derived in this work may not be the global optimum and further improvements in performance may be achievable with higher or lower

values. Default values, as defined in the BSM2 default closed loop control strategy (Nopens et al. 2010), represent the base case (note: despite being a useful reference point, this control strategy was designed only to provide a starting point for further development, and not to be optimal in any way).

Values of each decision variable for each individual in the initial population are selected randomly within the feasible range. To aid the optimisation process and ensure at least one ‘good’ solution in the initial population, the decision variable values of one individual are set to those of the base case.

Table 6.2: Decision variables for optimisation problem

Variable	Default (base case)	Optimisation range		Notes
		Min	Max	
Qintr (m ³ /d)	61,944	51,620	72,268	BSM2 default ± 10% of feasible range
Qw (m ³ /d)	300	93.5	506.5	BSM2 default ± 10% of feasible range
KLa1 (/d)	0	0	24	BSM2 default ± 10% of feasible range
KLa2 (/d)	0	0	24	BSM2 default ± 10% of feasible range
carb1 (m ³ /d)	2	1.5	2.5	BSM2 default ± 10% of feasible range
carb2 (m ³ /d)	0	0	0.5	BSM2 default ± 10% of feasible range
carb5 (m ³ /d)	0	0	0.5	BSM2 default ± 10% of feasible range
Controller setpoint (g/m ³)	2	0	10	Based on DO sensor range
Controller offset	120	0	240	Based on allowable <i>KLa</i> actuator range
Controller amplification	25	0	500	Arbitrary range to give appropriately scaled output
Controller integral time constant	0.002	0.0005	0.0035	Arbitrary range, centred on BSM2 default
KLa3 gain	1	0	1	Selected to ensure <i>KLa3</i> is within allowable actuator range
KLa5 gain	0.5	0	1	Selected to ensure <i>KLa5</i> is within allowable actuator range

Objectives and Constraints

Three different optimisation problem formulations with different objective sets are implemented in separate optimisation runs, in order to investigate the effectiveness of different approaches and to enable a comparison of the potential benefits achievable and the associated trade-offs. The objective sets for the three problem formulations are defined as follows:

- Set X:
 - 1. Minimise OCI
 - 2. Minimise total GHG emissions
- Set Y:
 - 1. Minimise OCI
 - 2. Minimise total GHG emissions
 - 3. Minimise EQI
- Set Z:
 - 1. Minimise OCI
 - 2. Minimise total GHG emissions
 - 3. Minimise BOD₅
 - 4. Minimise ammonia
 - 5. Minimise nitrogen

In each case, constraints are implemented for maximum effluent pollutant concentrations, to ensure compliance of solutions with the UWWTD. All constraints are implemented using a penalty function: if a solution is non-compliant with one or more constraints, all objective function outputs are increased by a factor of 100.

Objective set X aims to identify the greatest possible theoretical reduction in cost and GHG emissions whilst maintaining legislative compliance; however, performance with regards to effluent quality is likely to be poor and with little headroom for maintained compliance in the case of a significant change in influent. Objective sets Y and Z, therefore, also include measures of effluent quality, to allow analysis of the trade-offs. Objective set Y uses a single measure, EQI, to assess plant performance, since evolutionary multi-objective algorithms are inefficient with a large number of objectives and produce trade-offs which are hard to represent and difficult for a decision maker to consider (Deb and Jain 2012). However, a low EQI does not necessarily correspond with a compliant solution: therefore, performance assessment in objective set Z is

based directly on the UWWTD requirements. Minimisation of COD and TSS are not included as analysis of preliminary optimisation results shows a strong positive correlation between BOD₅ and COD, and effluent TSS is found not to be critical. Minimisation of ammonia is also included since, despite not being limited by the UWWTD, discharge consents commonly specify a limit; where applied, this is expected to be a critical factor given the slow rate of nitrification relative to organic removal.

Theoretically, GHG emissions could be represented as a cost, given that a charge of £15.60 per tonne on CO₂ is levied for carbon credits purchased in advance (for 2014-2015) (CHPA 2013). This approach would reduce the number of objectives, simplifying the problem and potentially enabling it to be addressed as a single-objective optimisation. However, this would not allow investigation into the trade-offs between operational costs and GHG emissions. Furthermore, operational costs are represented by an OCI rather than an absolute cost; combining emission credit costs would require appropriate unit conversions to assess the relative costs of each contributor.

Algorithm Parameters

It is necessary to achieve a balance between the number of simulations carried out and NSGA-II performance, given the high computational demand of the model. For each objective set, a setting of 25 generations with a population size of 500 (i.e. 500 solutions for evaluation in each generation), repeated 10 times, is found to be sufficient to derive the Pareto front. Further information on the convergence of multi-objective optimisation results is provided in Appendix B. A large population size is necessary to achieve good coverage of the Pareto front, and the optimisation process is repeated multiple times for each scenario as the randomised initial population leads to a different set of solutions in each instance. The results from each run are combined and non-dominated solutions selected.

A crossover probability of 0.9 and a mutation probability of $1/n$, where n is the number of decision variables, are selected.

6.1.3 Multi-Objective Optimisation Results

Optimal solutions derived using each objective set and an analysis of the associated trade-offs are presented in the following sections. Solutions enabling simultaneous reduction of GHG emissions and OCI whilst maintaining legislative compliance were found using each set, but no solutions also bettering the base case effluent quality were identified.

Minimising Greenhouse Gas Emissions and Operational Costs Whilst Retaining Compliance

The performance of the base case and non-dominated solutions derived using objective set *X* is presented in Figure 6.3. All solutions provide a reduction in both GHG emissions and OCI with respect to the base case and a maximum reduction of emissions of 18.5% is shown to be achievable with a corresponding 4.1% reduction in operational costs. There is a distinct trade-off between operational costs and GHG emissions, however, with the lowest emission solutions incurring the highest operational costs.

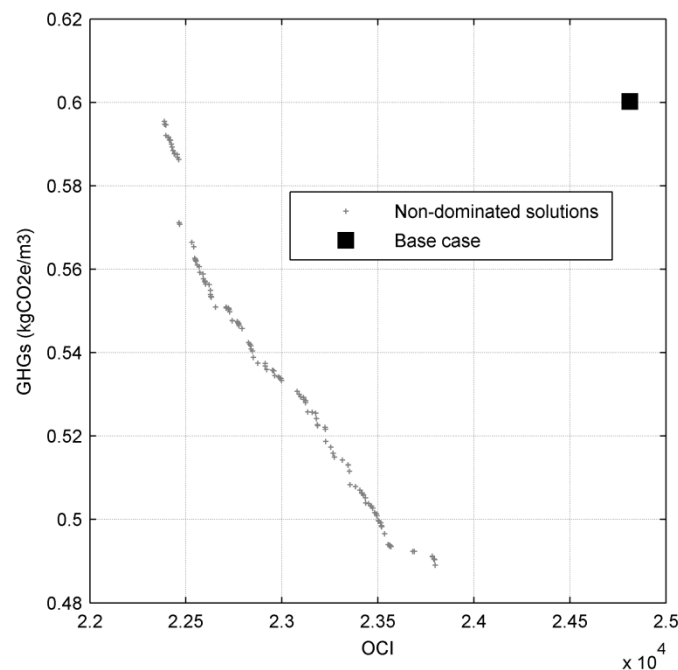


Figure 6.3: Performance of non-dominated solutions derived using objective set X, with regard to corresponding objective functions

Minimising Greenhouse Gas Emissions, Operational Costs and a Single Effluent Quality Measure

Performance of all non-dominated solutions derived using objective set Y, with regard to the corresponding objective functions, is shown in Figure 6.4 and solutions which better the base case in terms of both GHG emissions and OCI are identified (as illustrated by the dotted lines in Figure 6.4d). A reduction in GHG emissions of up to 18.8% is achievable without increasing costs, although the lowest emission solutions worsen the EQI.

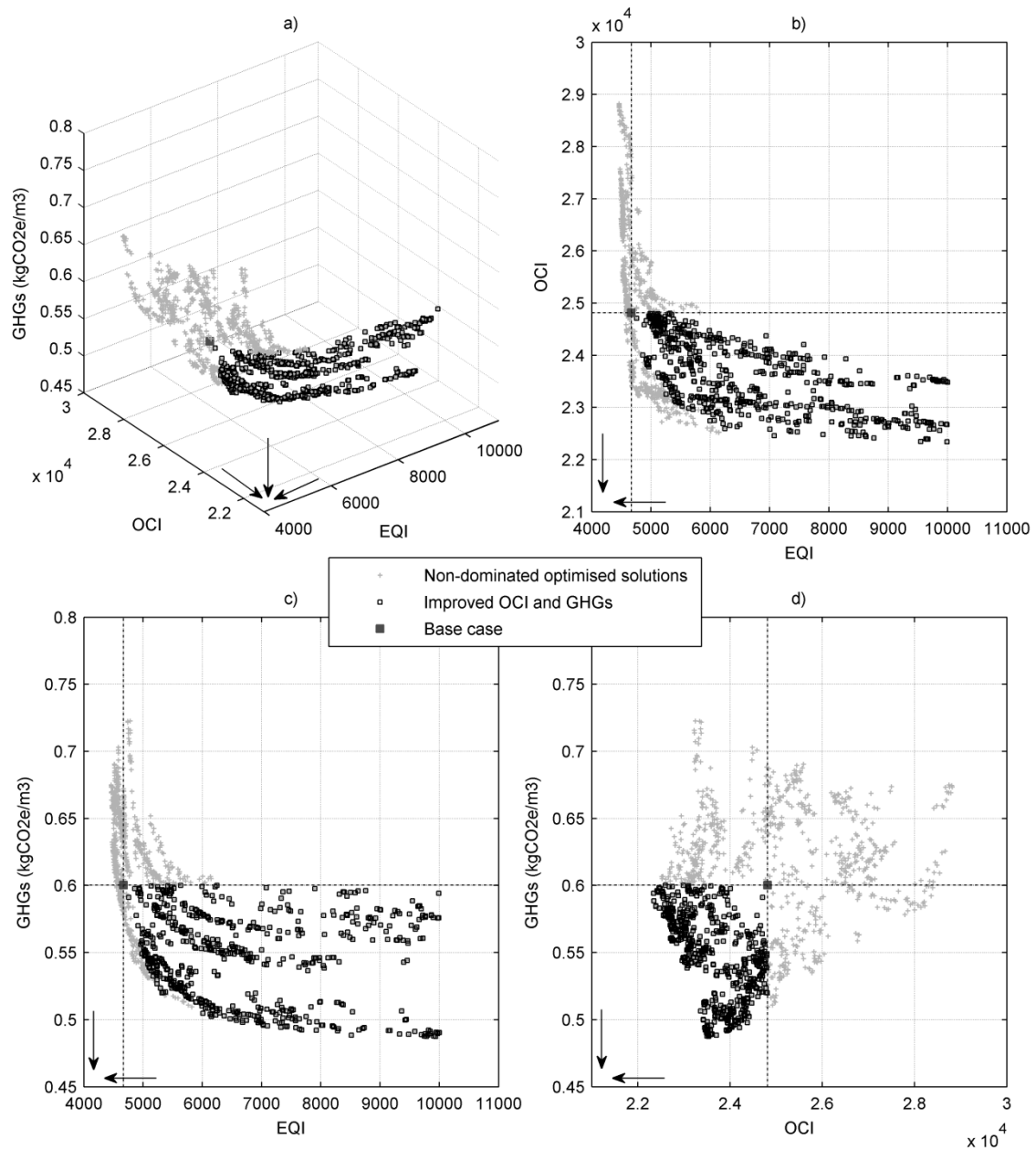


Figure 6.4: Performance of non-dominated solutions derived using objective set Y, with regard to corresponding objective functions

Figure 6.4c shows that few solutions enable a reduction in GHG emissions with little or no trade-off in effluent quality, and those that do result in an increase in operational costs. However, all solutions presented produce a compliant effluent and solutions enabling a reduction in GHG emissions with no additional operational costs are identifiable.

These results also highlight the importance of considering the effects on GHG emissions when developing control strategies: 87.6% of non-dominated solutions which improve the base case EQI also result in an increase in emissions, suggesting that if reduction of operating costs and improvement of effluent quality are prioritised in control strategy development, emissions may inadvertently be increased. This finding is supported by the results of scenario analysis by Flores-Alsina et al. (2011), in which a reduction in EQI was found to correspond with an increase in GHG emissions in several control strategies implemented.

Minimising Greenhouse Gas Emissions, Operational Costs and Specific Effluent Pollutant Loads

A pair-wise representation of the performance of all non-dominated solutions derived using objective set Z with regard to GHGs, OCI, BOD₅, ammonia and total nitrogen is given in Figure 6.5. Of the 2194 solutions presented, 28.9% better the base case GHG emissions and only 23.0% do so without increasing costs. The lowest cost solutions offer negligible reduction in GHG emissions; however, emissions can be reduced by up to 17.4% whilst also cutting the OCI by 3.6%.

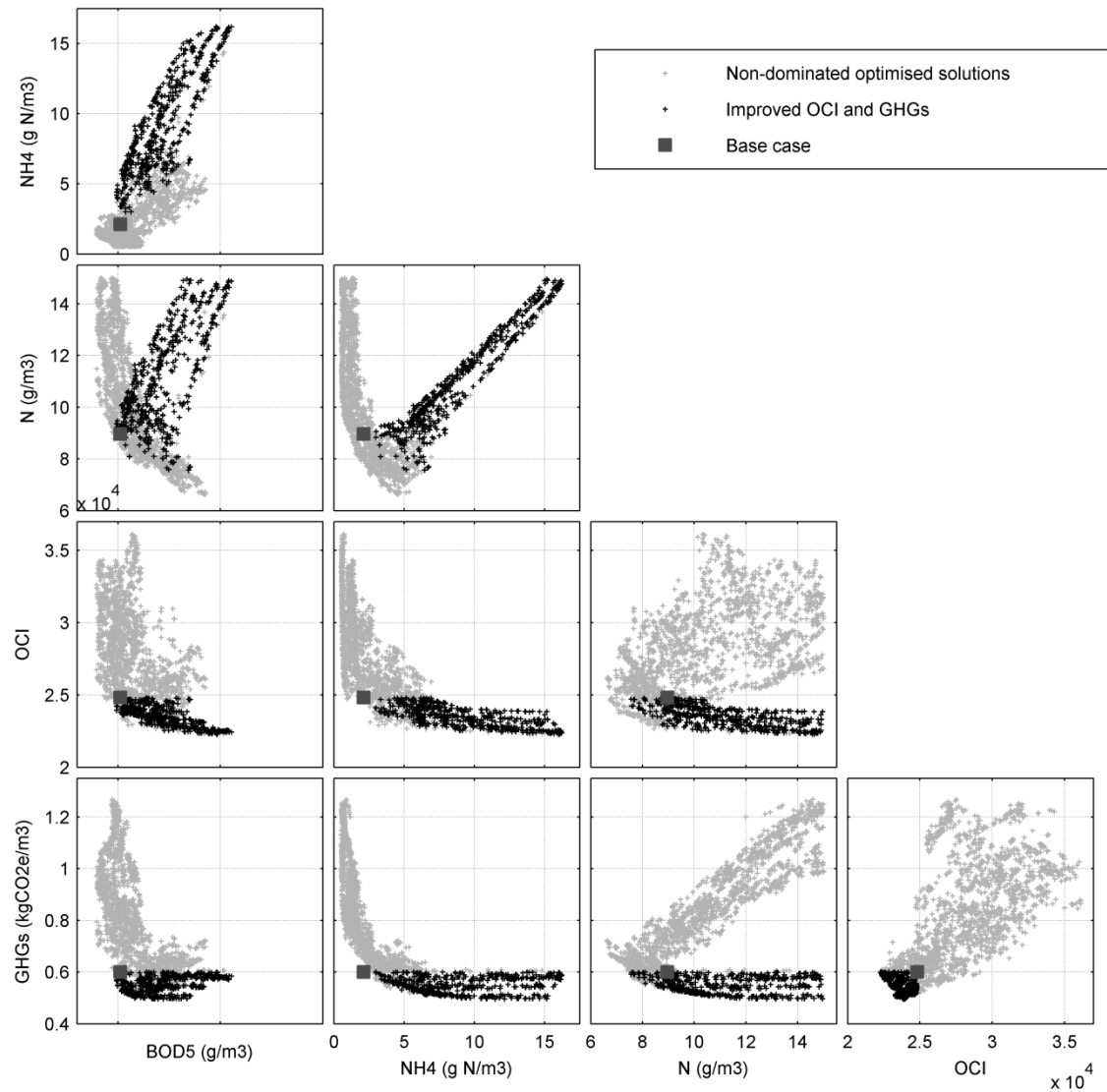


Figure 6.5: Performance of non-dominated solutions derived using objective set Z, with regard to GHGs, OCI, BOD_5 , ammonia and total nitrogen

The results suggest that, for the control loop studied, a reduction in GHG emissions and/or OCI corresponds with an increase in ammonia concentration – and, based on objective set Z, all optimal solutions which improve upon the base case ammonia concentration result in an increase in both GHG emissions and OCI. A strong correlation between ammonia and total nitrogen is also observed and 89.1% of solutions offering a reduction in GHG emissions and operating costs also increase total nitrogen, although UWWTD compliance is maintained in all cases. This corresponds with previous research (Flores-Alsina et al. 2011), in which adjustment of operational or control parameters to reduce GHG emissions resulted in a significant increase in ammonia and nitrogen time in violation. It is important to remember, however, that N_2O emissions resulting

from the nitrifier denitrification pathway (oxidation of ammonia to nitrate) are not modelled and, given the elevated ammonia concentrations, such emissions may be significant.

Non-dominated solutions which better the base case GHG emissions and/or OCI also typically increase the effluent BOD₅, although in all cases the BOD₅ is significantly below the limit for compliance.

For all effluent quality indicators used in the objective functions, the solutions providing the lowest pollutant levels increase GHG emissions with respect to base case performance, again highlighting the importance of including assessment of GHG emissions in the development of control strategies.

6.1.4 Performance and Legislative Compliance of Optimised Control Strategies

Further investigation is required to determine the extent to which it is necessary to compromise effluent quality if GHG emissions are to be reduced without incurring additional operational costs, and to identify the most effective objective set for optimising WWTP control to reduce GHG emissions whilst maintaining satisfactory effluent quality and costs. Due to the constraints set in optimisation, all control strategy solutions presented produce an effluent which is fully compliant with the requirements of the UWWTD during the evaluation periods considered; however, some solutions are close to breaching total nitrogen effluent limits and might not, therefore, remain compliant throughout an extended evaluation or under significant system disturbances. Figure 6.6, therefore, gives an overview of the distribution of total nitrogen performance for the sets of optimised control strategies from each objective set with respect to the UWWTD requirement, with the base case value indicated.

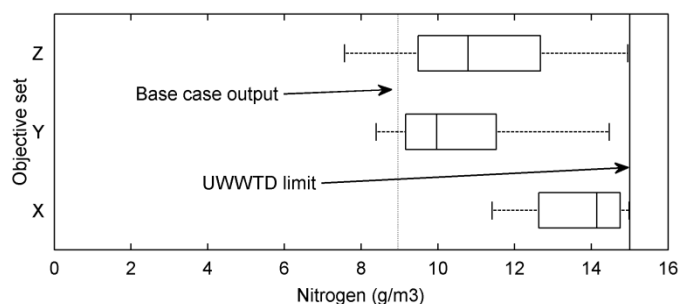


Figure 6.6: Performance distribution of optimised control strategies bettering base case GHG emissions and OCI

Each objective set results in a set of solutions which have a range of no more than 6% of the compliance limit and are less than 15%, 46% and 57% of the UWWTD limits for BOD₅, COD and TSS respectively. The most significant difference in the solutions derived using each objective set is in the nitrogen concentrations. Objective set X provides a set of solutions with the lowest GHG emissions and operating costs, but this is at the expense of elevated effluent nitrogen concentrations; over 50% of solutions produce an effluent with a safety margin of less than 6% of the UWWTD limit, suggesting that the likelihood of failure over an extended period is highest for solutions selected from this set. This may be attributed to highly optimised control strategies providing insufficient time and/or unsuitable conditions for adequate removal of nitrogen since, for example, bacteria responsible for nitrification of ammonia grow much more slowly than the heterotrophic bacteria responsible for removal of organic matter (Metcalf and Eddy 1994) and it is observed that, whilst BOD₅ concentrations are acceptable, ammonia contributes up to 84% of the high effluent total nitrogen. Optimising to minimise EQI (set Y) rather than individual effluent concentrations (set Z) gives the greatest proportion of solutions with a safety margin of at least 20%.

Overall, control strategy optimisation based on the minimisation of GHG emissions and operational costs alone, subject to legislative compliance, produces a set of solutions with the poorest effluent quality and the smallest safety margin. The wider spread of solutions derived from objective sets Y and Z is likely to be more useful to a decision maker, as these give more choice and allow for a more complete assessment of necessary trade-offs, depending on the case-specific priorities. Using a single index to represent effluent quality simplifies the comparison and selection of solutions, and it is shown that, for a fixed number of model evaluations, optimisation using objective set Y yields solutions of a similar or better standard (with regard to effluent quality) as those developed when specific pollutant loadings are minimised.

6.1.5 Optimal Solutions

To allow further exploration of control strategy features which contribute to an effective, efficient and low emission solution, and to demonstrate the effects of optimisation on dynamic performance, three control strategies are presented in this section (one derived from each objective set). In each case, a solution

providing a 10% reduction in GHG emissions without increasing the operational cost is selected. For objective set Y, the solution with the lowest EQI which fits these criteria is selected, and for objective set Z, the solution with the lowest nitrogen, since this is shown to be closest to the failure limit.

Performance indicators and optimised decision variables for each solution and the base case are shown in Figure 6.7. Decision variables are normalised within the optimisation range and performance indicators are normalised within the compliant range where applicable, else from zero to the maximum observed value.

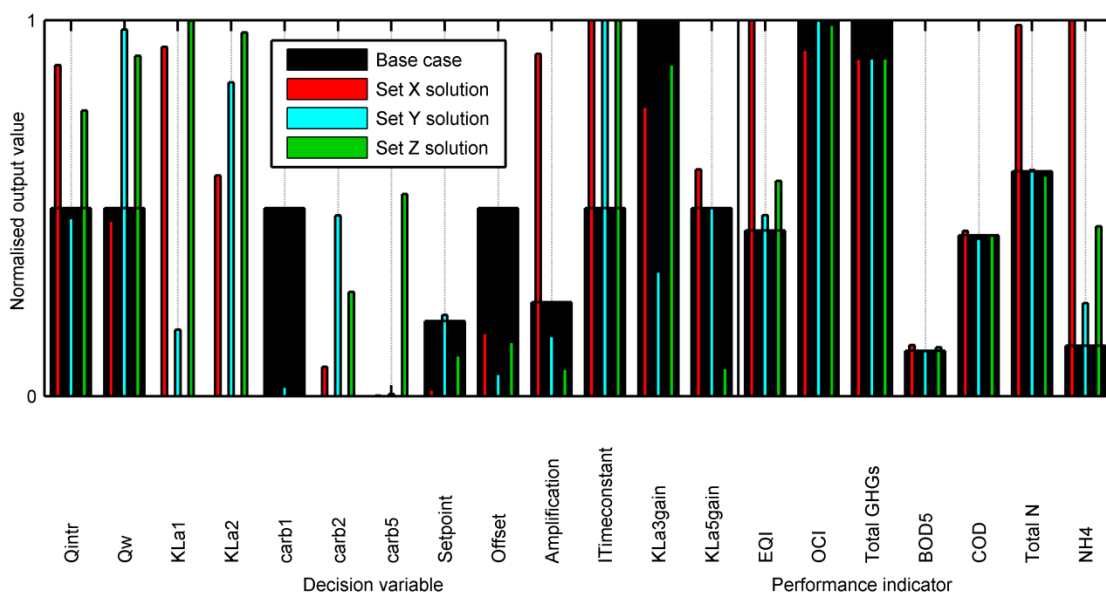


Figure 6.7: Decision variables and performance indicators for selected optimal solutions providing 10% reduction in GHG emission with no increase in OCI

Common features in the three optimised control strategies include:

- Introduction of a low level of aeration in the first two reactors, thereby creating aerobic conditions and removing the conventional anoxic zone
- Decrease in carbon source addition in the first reactor and an increase in the second (note that only static carbon source addition rates were considered; additional improvements may be achievable with dynamic control to reflect variations in the influent flow rate and carbon/nitrogen ratio deficiency)
- Reduction in controller offset (and therefore in aeration intensity in the fourth reactor)

- Reduction in KLa_{3gain} , and therefore in aeration intensity in the third reactor
- Increase of the controller integral time constant, resulting in a slower controller

Low level aeration in the anoxic zone is unconventional and may not represent operating practice, but optimisation may have led to solutions with smaller variation in DO concentrations of adjacent reactors since transition between anoxic and aerobic conditions is a key condition leading to N_2O emissions (Law et al. 2012b). Low aeration in the anoxic zone may occur naturally as a side effect of mixing and previous studies have assumed this to provide a KLa of 2 d^{-1} (Flores-Alsina et al. 2011); however this would not fully account for the aeration intensities of up to 24 d^{-1} in the optimised solutions. Reduction of aeration intensities in the aerobic reactors in optimised control strategies may be attributed to the contribution of aeration to GHG emissions due to the significant associated energy consumption (Fernandez et al. 2011) and effects on stripping of N_2O from solution (Law et al. 2012b).

Optimal values for *carb1* and the integral time constant are at or near the limits of their respective optimisation ranges, suggesting that the optimisation may have been restricted by a limited range of allowable values. As these ranges do not correspond with physical constraints, further improvements may be achievable with a lower *carb1* value and higher integral time constant. The lower limit for *carb1*, for example, is $1.5\text{ m}^3/\text{d}$, but it is possible that satisfactory performance can be achieved in this reduced WWTP with no external carbon source addition. The effect of allowing further increase in Q_w could also be an area for further investigation since values near the upper bound are used in some of the optimal solutions.

In addition to a 10% reduction in GHG emissions, the results of these changes include increases in EQI and ammonia in all cases. Implementation of the objective set X solution causes the greatest increase in EQI, due to its significantly elevated nitrogen and ammonia concentrations – solutions from objective sets Y and Z are able to provide the same emission reduction whilst maintaining a better effluent quality and not increasing costs; this supports the theory that multi-objective optimisation objectives should include minimisation of effluent pollutant loadings in addition to cost and emission considerations.

Representation of the pollutant loadings by a single measure (as in objective set Y) enables the required emission reduction to be achieved with no increase in cost and the smallest impact on effluent quality.

Analysis of the dynamic performance of these control strategies offers an insight into the source of overall performance variations. The rate of GHG emissions through both the summer and winter evaluation periods is shown in Figure 6.8. Dynamic effluent nitrogen and ammonia concentrations are also shown since these are of greatest concern and differ significantly between the solutions.

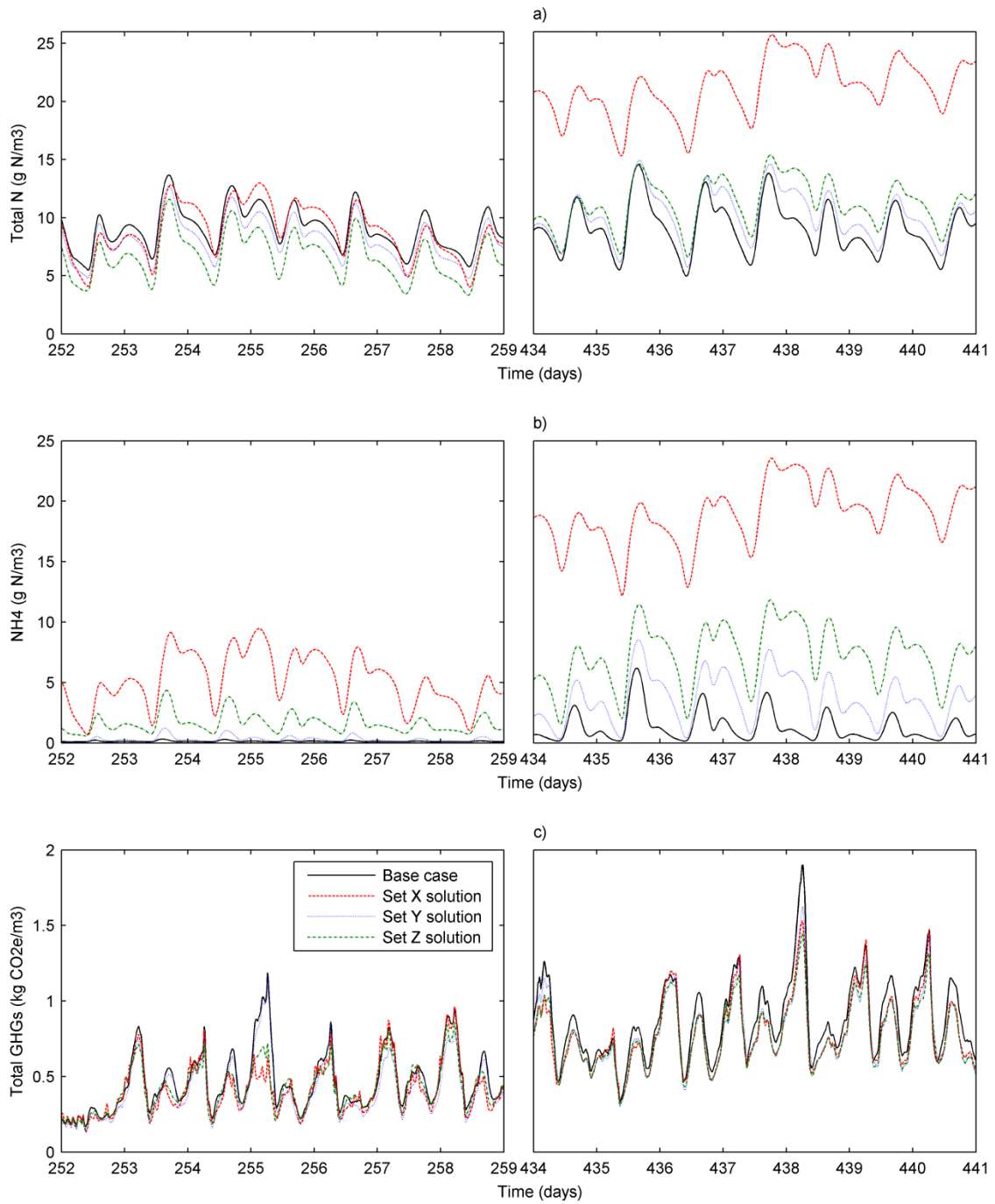


Figure 6.8: Dynamic performance of selected optimal control strategies with respect to nitrogen, ammonia and GHG emissions during the summer (days 252-259) and winter (434-441) evaluation periods

The rate of GHG emissions fluctuates significantly and is greatest during the winter period, but there is little to distinguish the control strategies. All three proposed strategies yield small but consistent improvements throughout, with some greater reductions observed at the points of peak emissions in the base case. On the basis of these results alone, no one control strategy is preferable, as all provide the required emission reduction. Analysis of the dynamic nitrogen

and ammonia concentrations, however, highlights the differences between the control strategies.

The departure in effluent quality from the base case values is most distinct in the winter period, and in particular for the set X solution. This is likely to be due to a combination of the reduced, optimised DO setpoints resulting in insufficient oxygen for nitrification and the lower temperature reducing the nitrifier growth rates. Over the winter period, when nitrogen and ammonia concentrations are higher, the solution from objective set Y consistently produces effluent with the lowest nitrogen and ammonia concentrations (of the optimised control strategies), reinforcing the theory that control strategy optimisation using a single indicator to represent effluent quality is preferable. Performance of the set X solution, optimised for just GHG emissions and operational cost, is likely to be unacceptable as nitrogen concentrations in the winter are greater than 15 g N/m^3 and, in one instance, exceed 25 g N/m^3 . Whilst this solution (just) complies with the UWWTD requirement for an annual mean total nitrogen concentration of less than 15 g N/m^3 based on the two evaluation periods considered, failure in an extended evaluation is highly likely.

6.1.6 Conclusions Drawn from Multi-Objective Optimisation Results

This research has demonstrated the potential of multi-objective optimisation of WWTP control strategies for the reduction of GHG emissions in a cost effective manner. Exploration of different problem formulations for the optimisation process, investigation into performance trade-offs and analysis of optimised solutions has led to the following key findings:

- Multi-objective optimisation of WWTP operational parameters and controller tuning parameters enables a significant reduction in GHG emissions without the need for plant redesign or modification of the control strategy layout.
- A large range of options are available for reducing GHG emissions without incurring additional operational costs which also maintain an acceptable effluent quality.
- GHG emissions may be reduced with no loss in effluent quality, but this is likely to incur increased operational costs.

- If operational costs are not to be increased, reduction of GHG emissions is likely to incur an increase in effluent nitrogen and ammonia concentrations.
- If control strategies are selected with a preference for high effluent quality and low costs alone, GHG emissions may be inadvertently increased. It is, therefore, of key importance that effects on emissions are considered in control strategy development and optimisation.
- When using multi-objective optimisation of control strategies to reduce GHG emissions, it is preferable to include minimisation of pollutant loadings in the objective functions. However, using a single index to represent effluent quality is more effective than optimising to minimise specific pollutants and simplifies comparison of optimal solutions.

6.2 Comparison of Different Control Strategies under Extended Performance Evaluation

Multi-objective optimisation has been used in Section 6.1 to obtain a clearer picture of the trade-offs between GHG emissions, operational costs and effluent quality. However, the results cannot be used to prescribe a specific control strategy that will provide a cost efficient reduction of GHG emissions, due to the use of a short simulation period and the potential for reduced performance when evaluated over a full year. Furthermore, only one control strategy is considered; further improvements achievable with alternative control strategies are not explored.

The objective of this section of research is to investigate the potential of improved control strategy design and parameterisation for the reduction of GHG emissions from WWTPs, taking into account the need to produce an acceptable effluent quality whilst remaining cost efficient and considering long term performance. Global optimisation of control strategies based on dynamic performance over an extended period is challenging due to the high computational demand of mechanistic WWTP models and large number of model evaluations required. In this study, therefore, two control strategies are considered and operational parameters to which GHG emissions, operational costs and effluent quality are found to be most sensitive are sampled using the

factorial sampling design approach to provide a search of the decision variable space.

6.2.1 Wastewater Treatment Plant Model, Simulation Strategy and Performance Assessment

Wastewater treatment processes and emission of GHGs are simulated in BSM2-e (full model, including sludge treatment), as detailed in Chapter 3. Simulations are carried out as in BSM2, using 200 days of constant influent to allow the model to reach steady state then 609 days of dynamic influent, of which the last 364 are used for evaluation. Given omissions in the sources of GHG emissions modelled (see Chapter 3), it is recommended that future work investigate the impact of control strategies developed in this study on such emissions since the net impact on emissions may be less desirable than anticipated. Again, it is important to note that the results obtained using this model are not directly comparable with those from BSM2 due to alteration of the activated sludge model.

6.2.2 Control Strategies

Activated Sludge Dissolved Oxygen Control

Maintaining an appropriate DO concentration in the activated sludge reactors is important in terms of its effects on GHG emissions: low DO concentrations result in slightly increased N_2O emissions due to incomplete denitrification and accumulation of NO_2^- , whereas high DO results in higher energy consumption in addition to increased N_2O resulting from incomplete nitrification (as DO is recirculated from the aerobic to the anoxic reactors) (Flores-Alsina et al. 2011). Sufficient DO must be supplied to maintain aerobic activity and avoid bulking issues, but over-aeration wastes energy since operating with DO close to saturation reduces the oxygen transfer efficiency. Excess DO can also result in poor biosolids settling and can affect nitrogen removal in the anoxic zone due to high levels of DO in the recycle flow (Spellman 2014).

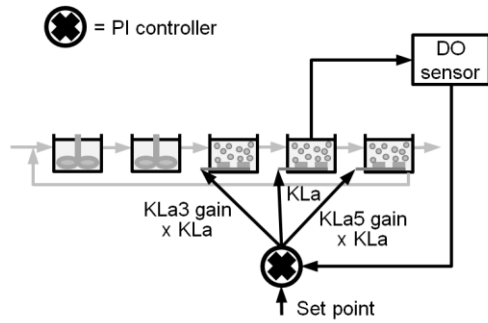
Oxygen demand fluctuates, due to variation in the influent and intermittent events such as dilution with stormwater or discharge of ammonia-rich supernatant from dewatering, and the efficiency of oxygen transfer varies with changes in temperature and wastewater characteristic. As such, the level of aeration necessary to maintain the required DO concentration also fluctuates.

To improve efficiency, therefore, DO concentration is commonly controlled using a feedback PI controller to manipulate aeration intensities, as in the BSM2 default closed loop control strategy (Section 3.7.2).

In this section, two different arrangements of sensors, controllers and actuators providing DO control are investigated, since it is known that DO control affects both operational costs (due to the impact on energy consumption (e.g. Åmand and Carlsson 2012)) and GHG emissions (e.g. Aboobakar et al. 2013). Sensitivity analysis has also shown aeration intensities in the aerobic activated sludge reactors to be key control handles for the reduction of GHG emissions, operational costs and effluent pollutant loadings (Sweetapple et al. 2014a).

Firstly, the BSM2 default closed loop (DCL) control strategy (Nopens et al. 2010) is implemented; and secondly, one in which the DO spatial distribution is controlled using three independent control loops (3-DO control strategy). Both are illustrated in Figure 6.9. The BSM2 DCL control strategy with default parameter values (Nopens et al. 2010) represents the base case. The 3-DO control strategy has previously been shown to provide an acceptable effluent quality at an acceptable cost (Vanrolleghem and Gillot 2002) and Guo et al. (2012a) found this strategy to provide the greatest reduction in N₂O emissions. Given that N₂O is a significant contributor to total GHG emissions from wastewater treatment and the source with greatest potential for improvement (Sweetapple et al. 2014a), it is thought that this control strategy may provide cost-efficient reduction of emissions. Provisionally, a setpoint of 1 g O₂/m³ and offset of 200 d⁻¹ (Vanrolleghem and Gillot 2002) is set for every controller in this strategy.

a) Default closed loop control strategy



b) 3-DO control strategy

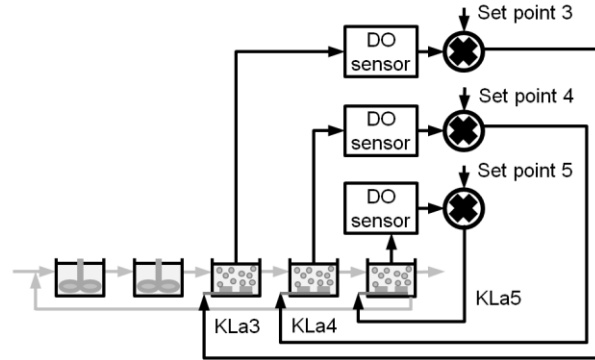


Figure 6.9: Control of the activated sludge unit in: a) the DCL control strategy; and b) the 3-DO control strategy

Activated Sludge Ammonium Control

Ammonium control may be implemented to maximise nitrogen removal and ensure complete nitrification. This can be achieved through cascaded control, using the DO setpoint as the manipulated variable (as illustrated in Figure 6.10), and has been implemented previously to reduce aeration costs whilst maintaining acceptable effluent quality (e.g. Flores-Alsina et al. 2008, Guerrero et al. 2012).

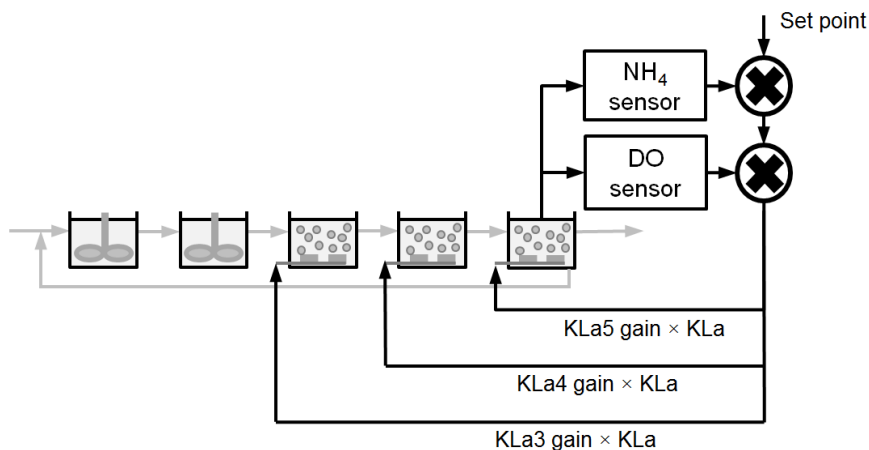


Figure 6.10: Cascade ammonium control

Previous attempts at control strategy optimisation (Section 6.1) found a high proportion of the optimal solutions to have excessively high ammonia and ammonium nitrogen concentrations, suggesting that ammonium control may be advantageous. This approach to improving effluent quality risks increasing GHG emissions, however, since it allows low DO concentrations when ammonium concentrations are low, which can result in high NO_2^- concentrations and in turn

promote production of N_2O by AOB (Guo et al. 2012b). For example, previous investigation (Flores-Alsina et al. 2011) found control with a cascade PI ammonium controller to manipulate the DO setpoint resulted in a 38% greater rate of N_2O emissions than control of DO using a simple PI loop with manipulation of aeration intensities. Although this effect can be mitigated by implementing minimum aeration intensities (e.g. Guo et al. 2012b), cascade ammonium control can also result in greater uncertainty in effluent quality than simpler alternatives when input uncertainty is considered (Flores-Alsina et al. 2008). Therefore, cascade ammonium control is not investigated further in this research.

Solids Retention Time Control

Selection of sensitive control handles for further adjustment in this study is based on the results of GSA using Sobol's method (Sobol 2001), which enables identification of significant individual and interaction effects (Chapter 5) as shown in Figure 6.11.

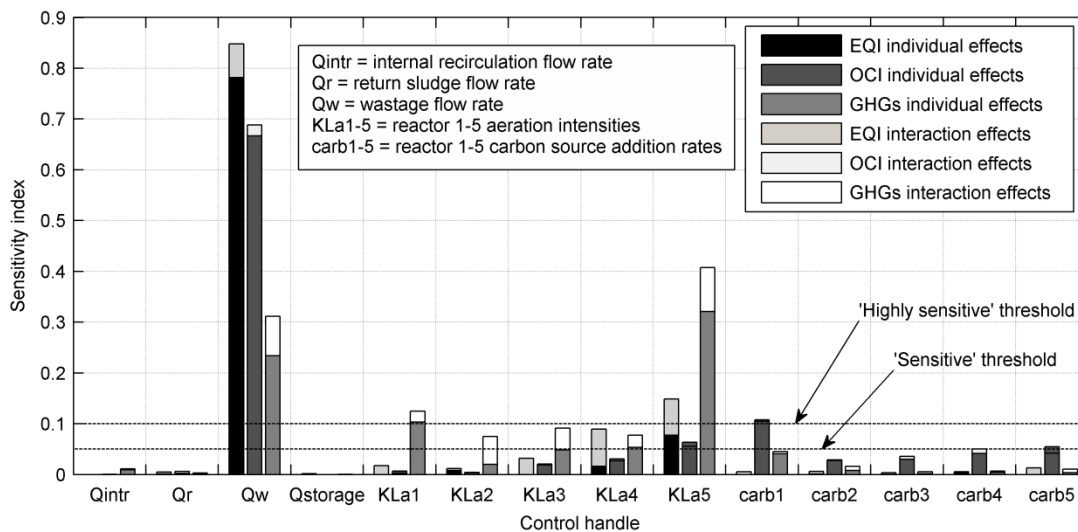


Figure 6.11: Sensitivity indices for WWTP operational parameters, calculated using Sobol's method, based on EQI, OCI and GHG emissions. Based on results in Chapter 5

GHG emissions, OCI and EQI are all shown to be highly sensitive to wastage flow rate (Q_w) and Flores-Alsina et al. (2011) have shown significant reduction in GHG emissions to be achievable by adjustment of Q_w to change the SRT, where high flow rate corresponds with a low SRT and vice versa.

The SRT represents the mean residence time of microorganisms in the reactor; only organisms that are able to reproduce within this time are retained in the system. Excessive wastage will prevent a stable population of bacteria developing if the SRT is less than that required (a particular issue for bacteria with a relatively low growth rate, e.g. autotrophic nitrifying bacteria), and washout may occur (Grady et al. 1999). However, insufficient wastage may result in problems such as increased DO demand, overloading of the clarifier and low F/M bulking (Ma and Peng 2006).

Control of SRT can considerably improve activated sludge performance by providing microorganisms with a stable environment and preventing filamentous bulking (Ma and Peng 2006). Traditionally, SRT is controlled by manual adjustment of the wastage flow rate, based on the mixed liquor suspended solids concentration or food-to-microorganism ratio. As WWTPs are subject to seasonal effects, optimal controller setpoints differ throughout the year (Stare et al. 2007) and reduced wastage flow rates may be implemented in order to maintain sufficient biomass in the system during winter months (e.g. Nopens et al. 2010, Flores-Alsina et al. 2011).

Automated SRT control can reduce variability in actual SRT and may be of particular benefit for overloaded or nutrient removal plants (Smith et al. 2014). However, it is not widely practiced, largely due to fear of the effects of a malfunction, and maintenance of online instrumentation has been found challenging (Smith et al. 2014). For the purposes of this study, therefore, automated SRT control is not considered, but manual adjustment based on temperature (and thus growth rate) is investigated.

It is decided to implement three different wastage rates (with values to be decided) in both control strategies throughout the year, dependent on temperature: QW_{low} (when $t \leq 13.2^{\circ}\text{C}$), QW_{medium} (when $13.2^{\circ}\text{C} < t \leq 16.8^{\circ}\text{C}$) and QW_{high} (when $t > 16.8^{\circ}\text{C}$). Limits are set so as to provide three equal width bands, based on the observed annual temperature range, as illustrated in Figure 6.12.

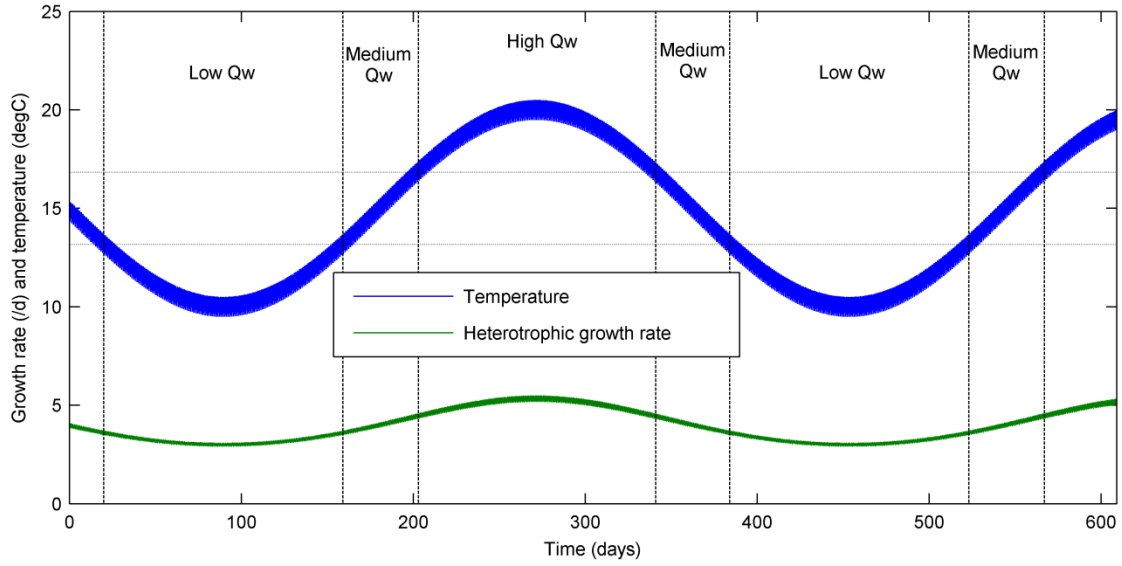


Figure 6.12: Influent temperature, modelled heterotrophic growth rate and proposed time frames for adjustment of Q_w

6.2.3 Selection of Operational Parameter Values

Factorial sampling is selected as it can provide good coverage of the search space within a relatively small number of simulations; Monte Carlo sampling, despite providing greater coverage, is not suitable due to the time taken for each model evaluation.

A 10-level factorial sampling design is used to generate a set of values for $Q_{w_{low}}$, $Q_{w_{medium}}$ and $Q_{w_{high}}$ within the range 93.5 to 506.5 m³/d for the OL and DCL control strategies. This contains 1,000 samples, reduced to 220 when instances in which $Q_{w_{low}} > Q_{w_{medium}}$ or $Q_{w_{medium}} > Q_{w_{high}}$ are removed. Samples evaluated in the 3-DO control strategy are restricted to 84 in which $Q_{w_{low}} > 139.5$ m³, since these were consistently found to produce a compliant effluent in the DCL control strategy.

Given that the control handle KLa_5 is also shown to be key for the reduction of GHG emissions and is classified as sensitive or highly sensitive based on all three performance indicators (Sweetapple et al. 2014a), the DO set point for reactor 5 in the 3-DO control strategy is also considered as a decision variable. This is sampled within the range 0.5 to 2.5 g O₂/m³ using 5-level factorial sampling for each combination of wastage flow rates.

6.2.4 Control Strategy Performance Results and Discussion

Wastage Flow Rate Adjustment

Performance of control strategies with adjusted wastage flow rates which produce a compliant effluent is shown in Figure 6.13 (complete results, including those providing a non-compliant effluent, are provided in Appendix C). It is observed that implementation of different combinations of Q_w values can enable a reduction of both GHG emissions and OCI simultaneously whilst maintaining compliance in each control strategy.

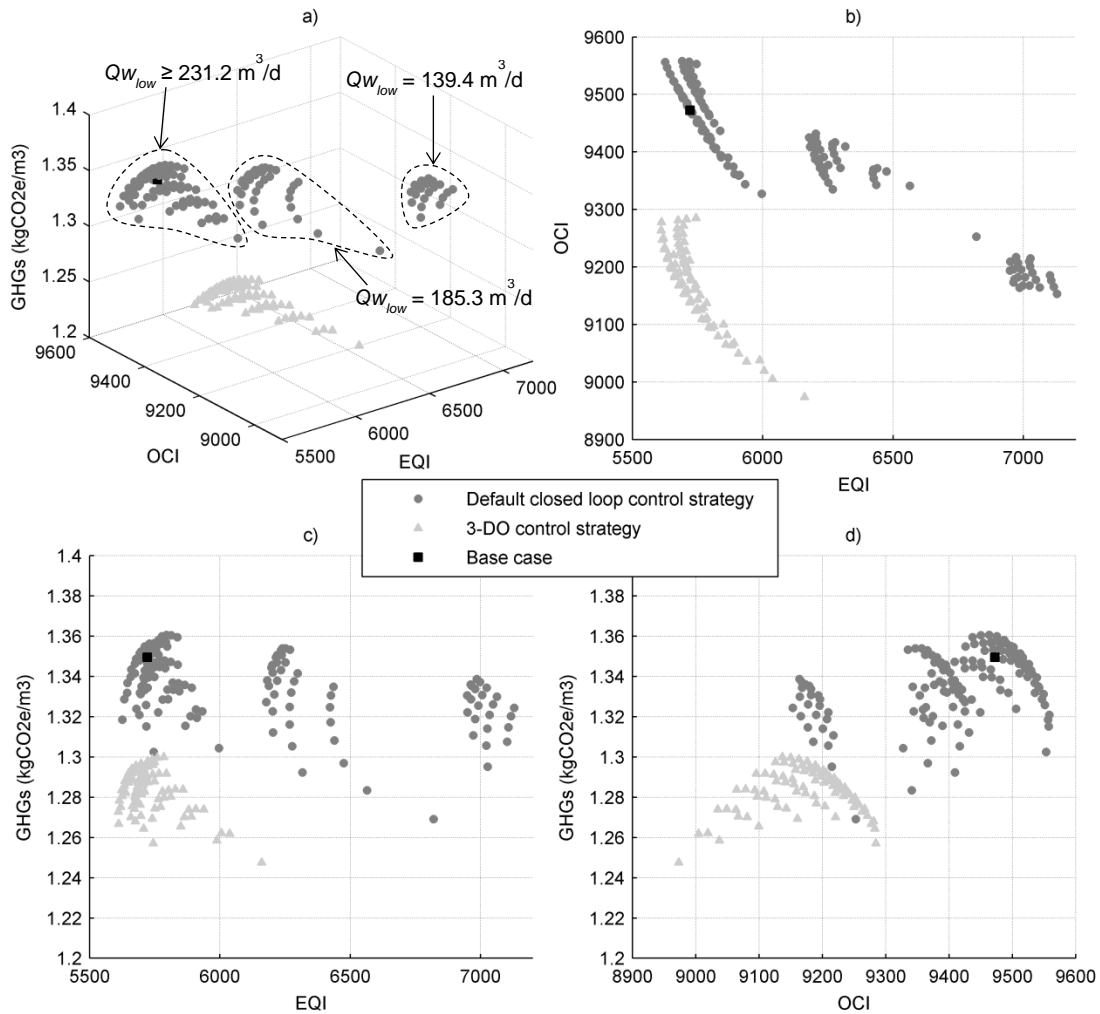


Figure 6.13: WWTP performance with adjusted control strategy wastage flow rates (compliant solutions only)

In the DCL control strategy, GHG emissions can be reduced by up to 6.0% with respect to the base case whilst also reducing the OCI by 2.3%. The lowest emission solution uses a constant wastage flow rate of $185.3 \text{ m}^3/\text{d}$ –

corresponding to a significantly longer SRT than in the base case (28 days mean compared with 15 days). The predominant source of reduction in operating costs is the reduction of sludge produced for disposal, not reduction in pumping costs as may be expected. Energy costs actually increase due to increased aeration requirements to maintain the specified setpoint. Reduction in GHG emissions associated with a reduction in energy required for pumping is also negligible (0.1% contribution). Change in N₂O emissions from the activated sludge reactors provide 131% of the net reduction in emissions whilst non-N₂O emissions from the activated sludge reactors provide -61% (i.e. they increase). This supports the observation of Flores-Alsina et al. (2011) that a high SRT increases direct non-N₂O emissions from the bioreactor and indirect emissions resulting from electricity use.

The reduction in GHG emissions and OCI achievable by adjustment of wastage flow rate in the DCL control strategy also corresponds with an increase in EQI (although all solutions presented remain compliant, and in some instances the impact on effluent quality is minor); all solutions which reduce the EQI increase operational costs. GHG emissions and EQI can be reduced simultaneously through improved control of wastage flow rates, but this is at the expense of OCI.

Solutions in the 3-DO control strategy have significantly lower GHG emissions and operating costs than those with a comparable effluent quality in the DCL control strategy. This highlights the importance of evaluating a range of alternative control options and suggests that, of the two DO control options studied, the 3-DO control strategy offers superior performance with regard to GHG emissions, operational costs and effluent quality. It also supports recommendation that implementation of the 3-DO control strategy would be economically wise (Vanrolleghem and Gillot 2002).

Using the 3-DO control strategy, an equivalent effluent quality to that of the base case can be maintained whilst reducing GHG emissions by 6.3% and also cutting operational costs by 2.0%, by implementing wastage flow rates of 231.2, 231.2 and 277.1 m³/d for $Q_{W_{low}}$, $Q_{W_{medium}}$ and $Q_{W_{high}}$ respectively. This solution provides a mean SRT of 22 days – again, significantly greater than that of the base case.

It may be thought that selection of a control strategy in which energy recovery from biogas combustion is reduced would be undesirable in terms of both operational costs and GHG emissions. This specific solution, however, exhibits a net decrease in both OCI and GHG emissions despite enabling less energy recovery than the base case control strategy: the increase in operational costs as a result of reduced energy recovery is less than the cost saving resulting from reduced sludge production, and the total indirect emissions resulting from net energy import decrease due to the reduction in energy required for pumping and aeration.

It is also found that implementing solutions providing a shorter SRT can be of benefit with regard to cost and emissions: the solution providing the greatest emission reduction (7.6%) in the 3-DO control strategy has a constant Q_w value of 506 m³/d (upper limit of range tested) and a mean SRT of 11 days and provides a reduction in both N₂O and non-N₂O emissions from the activated sludge unit. However, this also causes a 7.7% increase in EQI.

These contrasting combinations of Q_w values shown to provide a reduction in net GHGs with no additional operational costs demonstrate that an emission reduction is achievable with different approaches to SRT control, each of which affects different sources of emissions. Given the trade-off in EQI observed with a high wastage flow rates, however, it is suggested that a high SRT solution may be preferable. Furthermore, emissions not included in this study are likely to be significant in low SRT solutions: for example, N₂O emissions from biological hydroxylamine oxidation occur mainly at high NH₄⁺ and low NO₂⁻ concentrations (Wunderlin et al. 2012), which are likely to be present with a low SRT.

Dissolved Oxygen Setpoint Adjustment

Figure 6.14 shows that adjustment of DO concentrations in the final aerobic reactor (by manipulation of the DO setpoint) in addition to Q_w enables the development of solutions which further improve upon the base case GHG emissions and OCI whilst having negligible impact on effluent quality. Conversely, selection of too high a setpoint is found to increase GHG emissions and OCI.

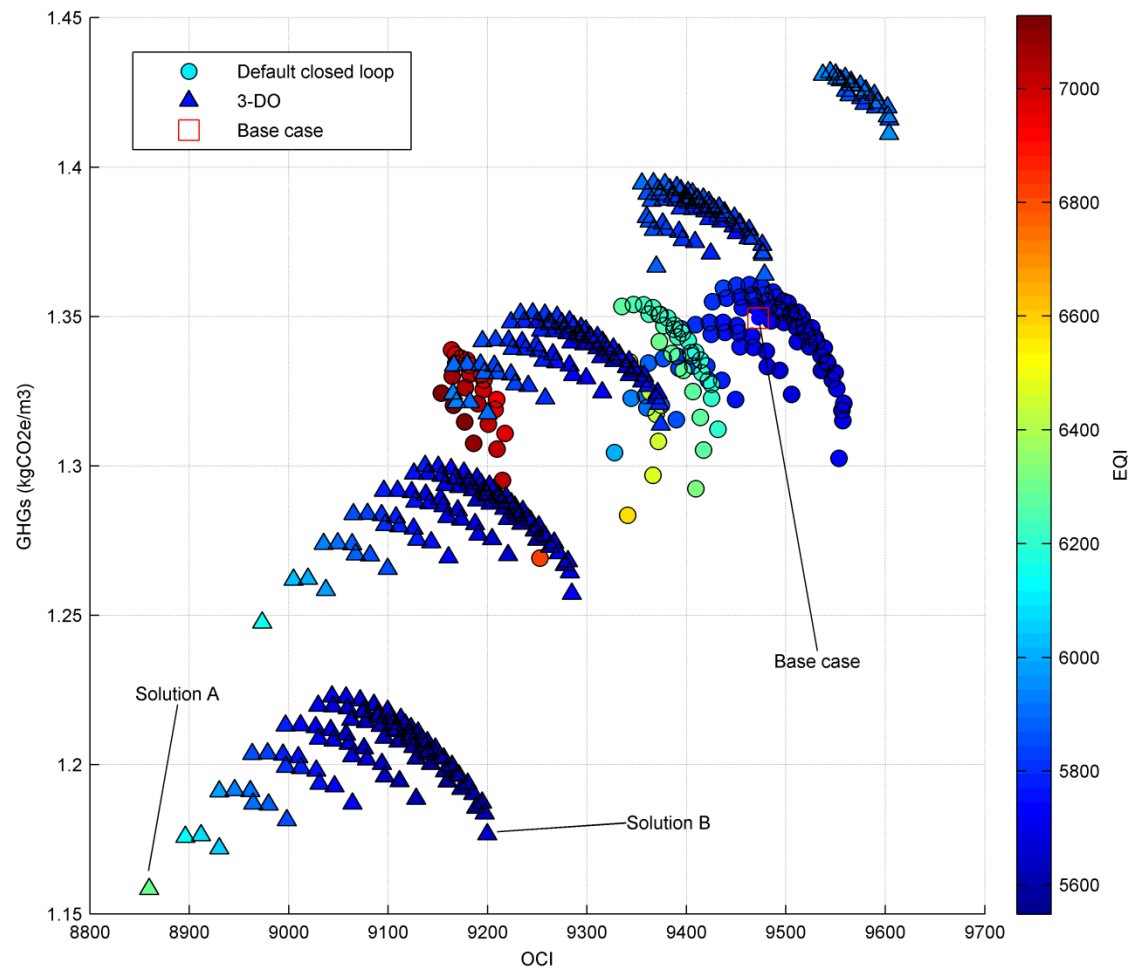


Figure 6.14: WWTP performance with adjusted reactor 5 DO setpoint in the 3-DO control strategy and adjusted wastage flow rates in 3-DO and DCL control strategies (compliant solutions only); colour denotes EQI

The cluster of solutions found to perform best with regard to OCI and GHG emissions all have a reduced DO setpoint of $0.5 \text{ g O}_2/\text{m}^3$. To enable analysis of the effects of Q_w adjustments on different contributors to operational costs and GHG emissions, two solutions in this cluster are compared in Table 6.3: Solution A provides the lowest GHG emissions and OCI but at the expense of effluent quality, solution B provides a smaller (but still significant) emission and cost reduction with respect to the base case but with no loss in effluent quality.

Table 6.3: Comparison of solutions, with percentage contribution of component change to total change in performance indicator in brackets. Only GHG and OCl components of interest are shown. Components worsened with respect to the base case are highlighted.

Solution		Base case	A	B
Aeration control		DCL	3-DO	3-DO
Mean SRT (days)		15.5	11.4	23.2
GHG components (kg CO ₂ e/m ³)	N ₂ O from activated sludge	0.50	0.34 (83%)	0.31 (111%)
	Non-N ₂ O from activated sludge	0.39	0.35 (20%)	0.43 (-24%)
	Pumping energy	0.01	0.01 (0%)	0.01 (0%)
	Aeration energy	0.05	0.04 (4%)	0.05 (1%)
	Sludge transportation and degradation	0.05	0.06 (-1%)	0.05 (2%)
OCl components (-)	Energy use	5560	4975 (95%)	5369 (70%)
	Energy recovery	-6425	-6693 (44%)	-6089 (-123%)
	Sludge for disposal	7938	8178 (-39%)	7519 (153%)
Performance indicators	Total GHGs (kg CO ₂ e/m ³)	1.35	1.16	1.18
	OCl	9472	8860	9200
	EQI	5722	6298	5670

In solution A, the cost reduction is achieved primarily through a reduction in energy use and an increase in energy recovery. Solution B, however, provides significantly less energy recovery than the base case yet still offers a reduction in overall operational costs and GHG emissions and an improved effluent quality. This again suggests that solutions providing the greatest energy recovery from biogas production may not necessarily be the most desirable in terms of net benefits.

As with the DCL control strategy, a high SRT solution results in an increase in non-N₂O emissions from the activated sludge but this is offset by the decrease in N₂O emissions to give a net reduction. Given that variance in direct N₂O emissions resulting from model parameter uncertainties is the greatest contributor to uncertainty in total GHG emissions (Sweetapple et al. 2013), it is suggested that reduction of N₂O emissions should be prioritised over reduction of non-N₂O emissions (as achieved with a high SRT approach).

In both cases, the reduction in N₂O emitted from the activated sludge units under reduced DO conditions is significant. This is as expected, since

denitrification enzymes, in particular those responsible for converting N_2O to N_2 , can be inhibited by the presence of oxygen, thereby preventing complete denitrification and resulting in emission of N_2O (Aboobakar et al. 2013). However, dynamic DO concentrations and total N_2O emissions are plotted in Figure 6.15 and no clear relationship between DO and N_2O emission is observed; DO fluctuations under the base case control strategy do not correspond with fluctuations in N_2O emissions, and solution B has lower N_2O emissions than solution A despite having near identical DO concentrations. This suggests that enzyme inhibition in the base case control strategy is not the primary cause of increased N_2O emissions. Instead, a clear correlation with flow rate (Figure 6.15c) is noted, as peaks in the rate of N_2O emissions correspond with a drop in flow rate.

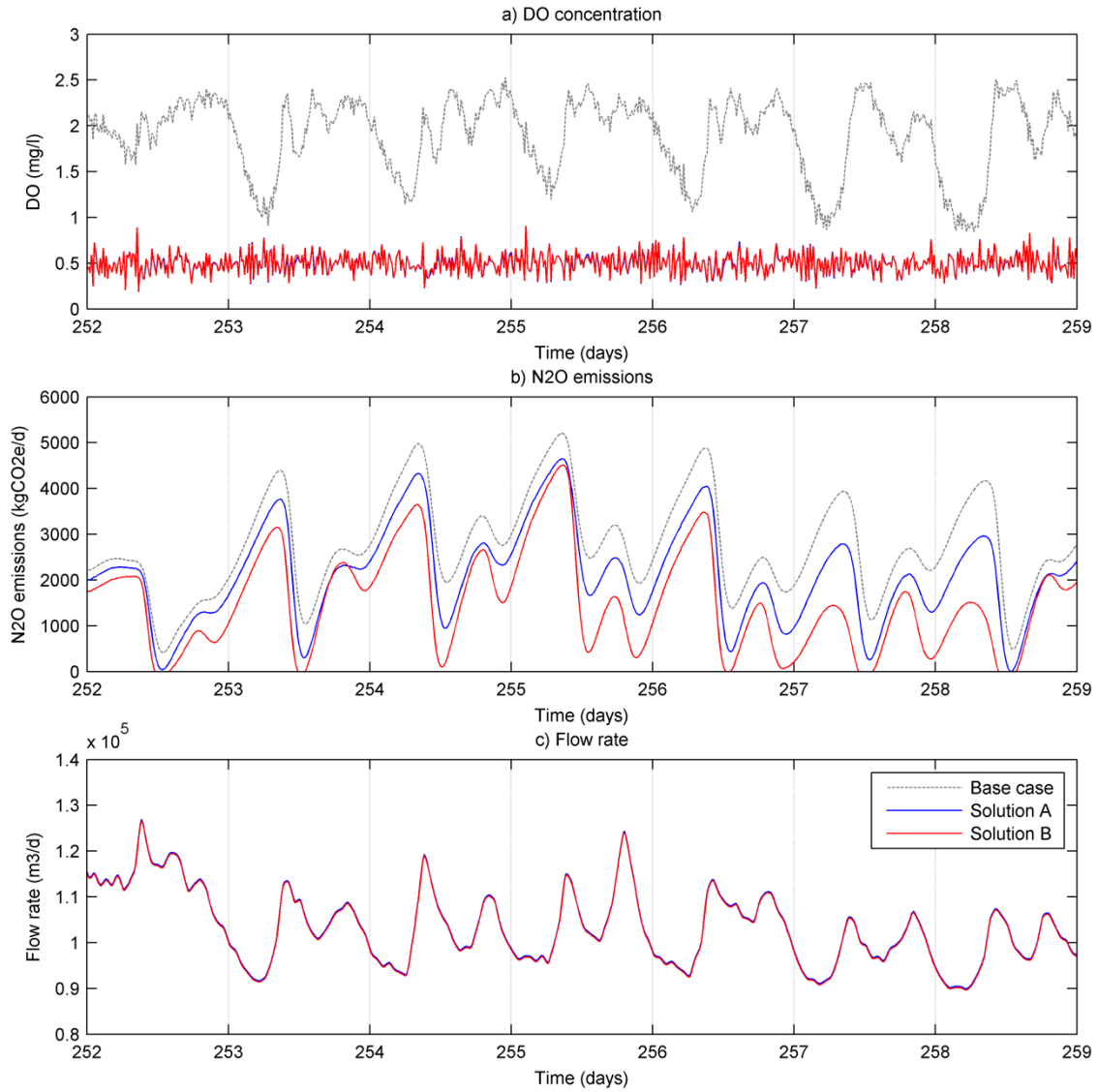


Figure 6.15: Comparison of dynamic N₂O emissions, DO concentration and flow rates in reactor 5 under solution A, solution B and base case control (one week displayed)

It is important to note that BSM2-e does not include modelling of N₂O emissions resulting from AOB denitrification, which are greatest in low DO conditions (Ni et al. 2013) as insufficient oxygen supply results in reduction of NO₂⁻ to N₂O instead of oxidation to NO₃⁻ (Aboobakar et al. 2013). It has been suggested that a DO concentration of at least 0.5 g O₂/m³ should be maintained to minimise N₂O emissions from nitrification (in which AOB denitrification plays a role) (Zheng et al. 1994). Figure 6.15a shows that DO under control strategies A and B fluctuates around the 0.5 g O₂/m³ setpoint, but it drops as low as 0.06 g O₂/m³ during the one-year evaluation period. As such, it is expected that N₂O emissions from nitrification will occur, despite not being modelled, but their

significance is uncertain. If reduced DO setpoints are implemented to reduce GHG emissions, therefore, a minimum setpoint of $0.5 \text{ g O}_2/\text{m}^3$ should be applied and either further modelling or monitoring undertaken to ascertain the effect on total GHG emissions.

6.2.5 Conclusions Drawn from Control Strategy Comparison

This study has investigated WWTP performance with regard to GHG emissions, operational costs and effluent quality under two different control strategies and with a range of wastage flow rates and DO setpoints. It is found that independent control of aeration in each aerated activated sludge reactor, in particular when using a low reactor 5 DO setpoint, enables significant reduction in both GHG emissions and operational costs whilst maintaining a high effluent quality. However, in both control strategies analysed, significant improvements can be achieved through better control of wastage flow rates alone.

The results emphasise the importance of considering the effects of emission reduction measures on emissions from a range of different sources rather than focussing on just one high priority source. Increasing the SRT, for example, can result in net emission and cost reduction but direct non-N₂O emissions are increased. Furthermore, it is suggested that developing control strategies to provide the greatest possible energy recovery may not always be necessary (or desirable) with regard to reducing GHG emissions and operational costs, since the effects of reduced energy recovery can be offset by the reduction in cost and emissions associated with sludge disposal, and a better effluent quality may be achieved.

6.3 Impact of Control Strategy Design to Reduce Total Greenhouse Gas Emissions on Emissions Resulting from Energy Consumption

Given that, under the Carbon Reduction Commitment (CRC), water companies are only required to measure and report their annual GHG emissions from energy supplies (rather than total GHG emissions), it is important to investigate the effects of developing control strategies to reduce total GHG emissions on energy related emissions. Therefore, sources of GHG emissions resulting from solutions and control strategies developed using both multi-objective optimisation of the reduced WWTP model (Section 6.1) and sampling of

wastage flow rates and reactor 5 setpoint in the full WWTP model (Section 6.2) are analysed.

6.3.1 Analysis of Optimised Control Strategy Solutions

Percentage reductions in energy related GHG emissions and in total GHG emissions for optimised solutions derived using objective set Y are presented in Figure 6.16. Only solutions which better the base case OCI and total GHG emissions are shown, and the corresponding EQI of each solution is represented with a colour scale.

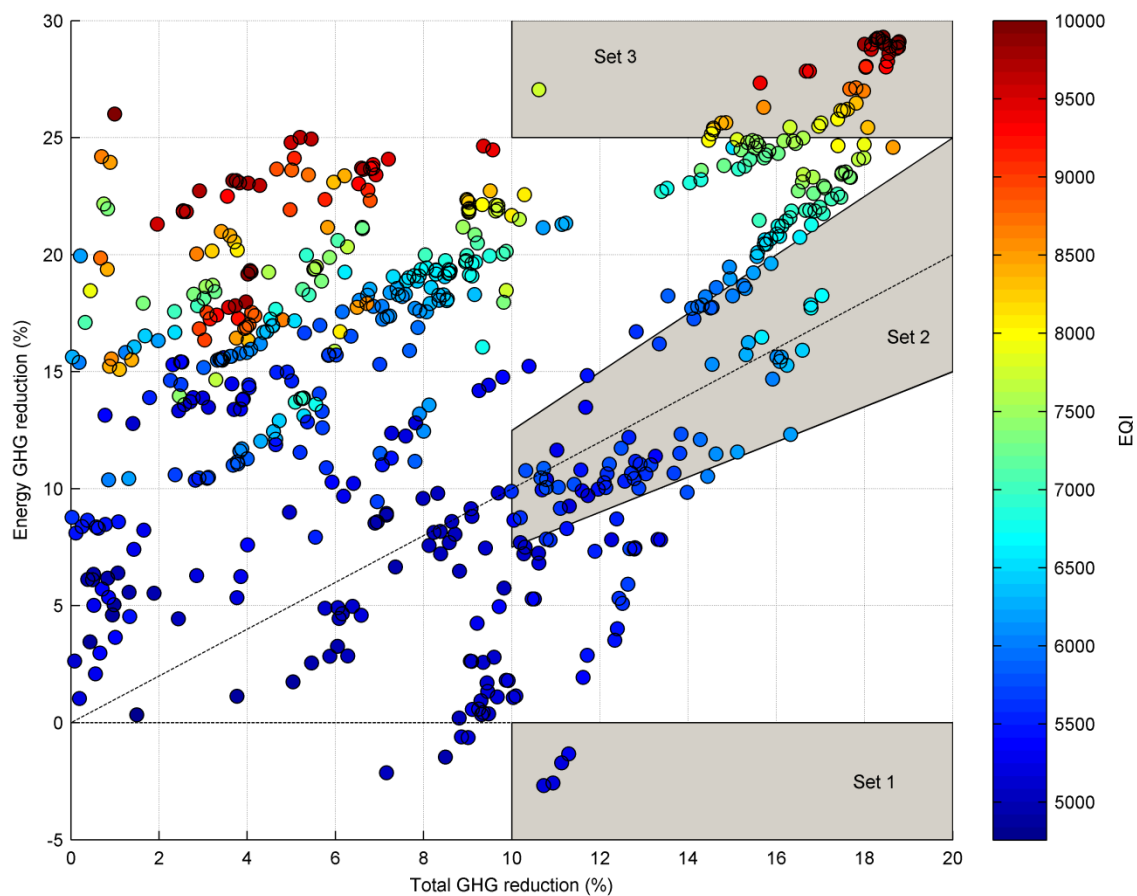


Figure 6.16: Comparison of percentage reduction in total GHG emissions and percentage reduction in GHG emissions associated with energy use with respect to base case (objective set Y solutions)

Of the 593 solutions shown in Figure 6.16 providing a reduction in total GHG emissions, 99% also reduce energy related emissions, although for 19% the percentage reduction is less than for total emissions. Typically, the solutions providing the greatest reduction in energy related emissions have the highest EQI so are undesirable from an effluent quality perspective, despite achieving

compliance during the evaluation period. Solutions which provide a percentage reduction in emissions from energy use which is equal to or less than that of total GHG emissions all yield a relatively good effluent quality (maximum EQI of 6467 and a mean of 5398).

Many solutions which provide a significant reduction in emissions resulting from energy use (and would, therefore, be highly desirable under the CRC), provide very little benefit in terms of net emission reduction. For example, there are solutions which reduce energy related emission by more than 20% (albeit with a severely compromised effluent quality) but reduce total GHG emissions by less than 1%. This shows that, despite the CRC incentivising reduction of GHG emissions resulting from energy use only, it is vital to consider the overall effect of any changes if real benefits are to be achieved.

To identify features of the optimised solutions which are common for solutions providing a similar reduction in energy related GHG emissions, three sets of solutions which provide a total GHG emission reduction of at least 10% (as identified in Figure 6.16) are analysed:

- **Set 1** contains solutions which increase energy related GHG emissions.
- **Set 2** contains solutions which provide a similar percentage reduction in both total GHG emissions and energy related GHG emissions (ratio of percentage reduction in energy GHG emissions to total GHG emissions in the range 0.75-1.25).
- **Set 3** contains solutions which provide a reduction in energy related GHG emissions of at least 25%.

Decision variable values and performance indicators for solutions in each set are presented in Figure 6.17. Decision variable values are normalised within the optimisation range (Table 6.2), whilst performance indicators are normalised from zero to the maximum observed value.

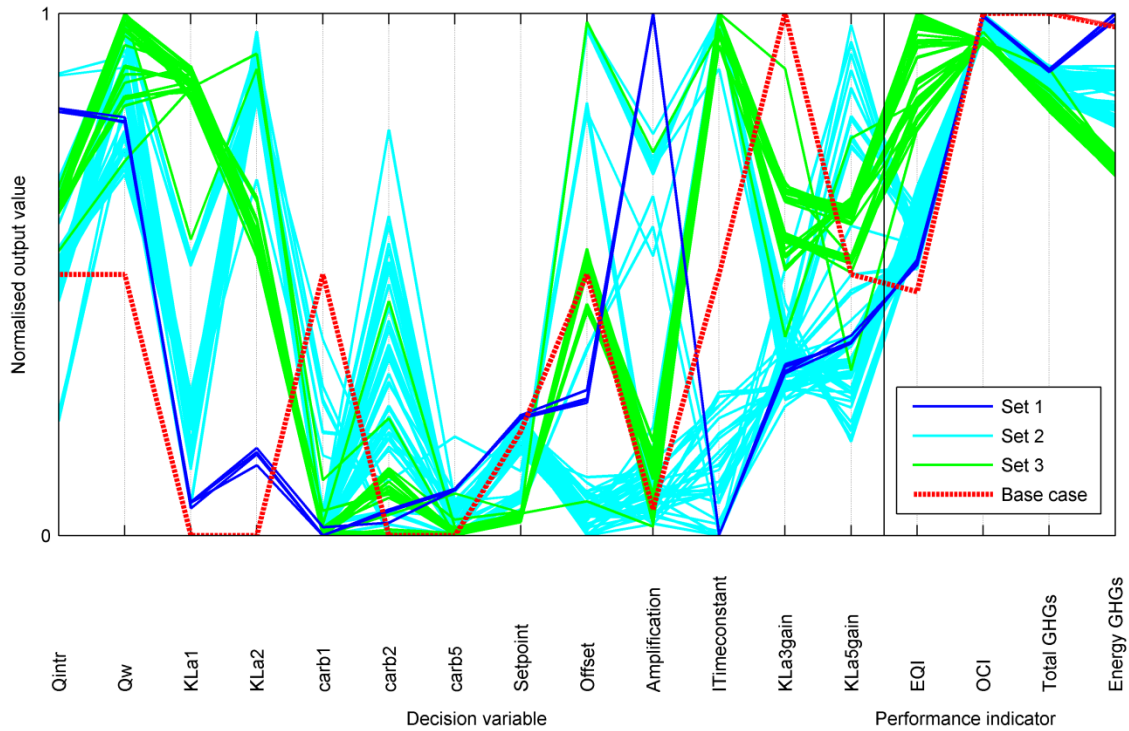


Figure 6.17: Decision variable and performance indicator values for solutions in sets 1, 2 and 3

Clear distinctions are visible between the $KLa1$, $KLa2$ and DO setpoint values for each solution set, showing that differences in energy use under different operational regimes are largely attributable to operation of the aerators. This knowledge is not new, however, and attempts at reducing operational costs due to energy use are commonly centred on improved DO control and increased aeration efficiency (e.g. Stare et al. 2007, Fernandez et al. 2011).

Solution sets 1 and 2 provide the best effluent quality (with EQI ranges of 5176-5285 and 5103-6679 respectively); this corresponds with the lower $KLa1$ and higher DO setpoint values with respect to solution set 3, which represent more conventional operating practices. Solutions in set 3, on the other hand, achieve significant reduction in energy related GHG emissions with a very low DO set point, but this also results in a poor effluent quality (EQI of at least 7752). This is expected since insufficient oxygen results in reduced nitrification and an increase in effluent ammonia (Galluzzo et al. 2001).

Implementation of solutions in set 1 would be regarded as bad under the CRC, yet when taking a holistic view they should be considered as desirable given the net impact on GHG emissions and ability to produce a high quality effluent.

Solutions in set 3 are desirable in terms of their emission reduction (both total emissions and energy related emissions), but they are unlikely to be given serious consideration given their severely compromised effluent quality and uncertain reliability over an extended period. In practice, solutions in set 2 are likely to be preferable since they offer significant improvements under the CRC requirements, reduce total GHG emissions and maintain a good quality effluent.

6.3.2 Analysis of Alternative Control Strategies

Performance of control strategy solutions derived through sampling of wastage flow rates in the DCO and 3-DO control strategies and of the reactor 5 setpoint in the 3-DO control strategy, with respect to their total GHG emissions and emissions resulting from energy use, is presented in Figure 6.18. Solutions A and B identified are those discussed in Section 6.2.4.

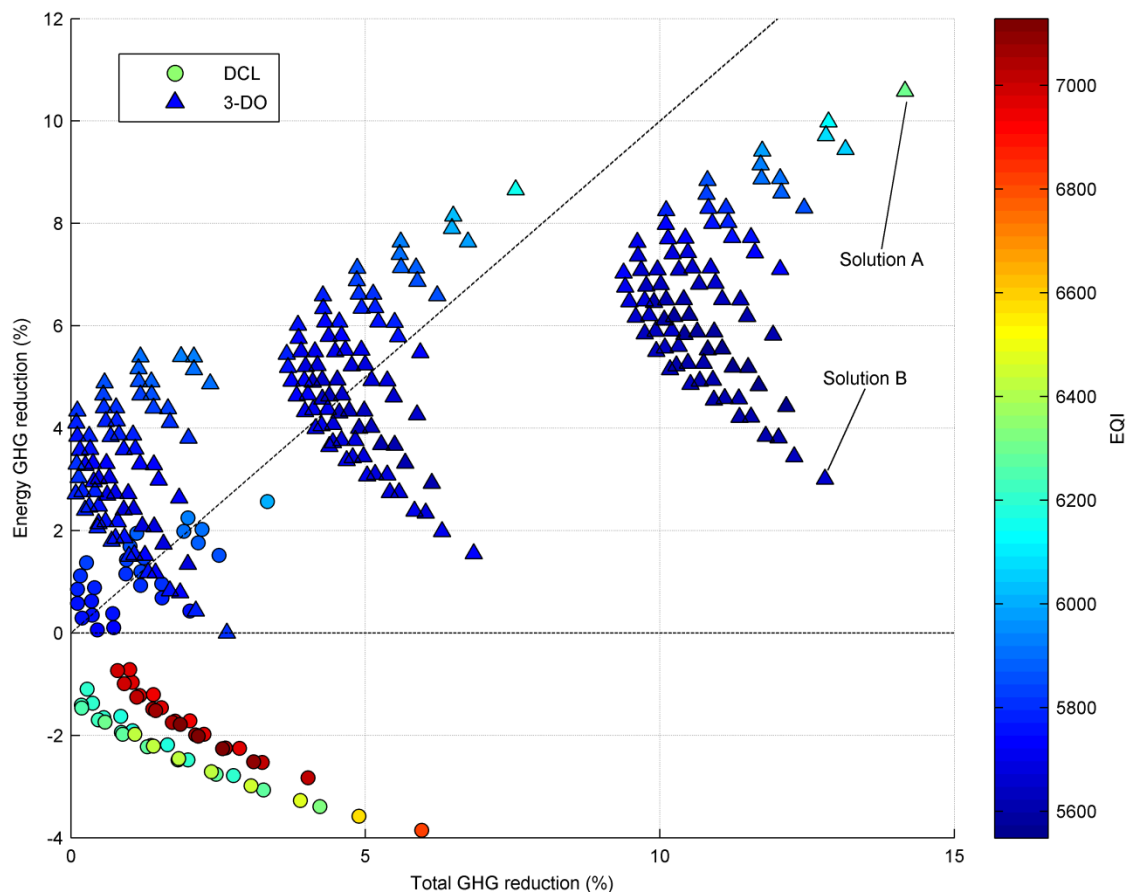


Figure 6.18 Comparison of percentage reduction in total GHG emissions and percentage reduction in GHG emissions associated with energy use with respect to base case, for solutions in 3-DO and DCL control strategies which improve upon base case OCI and GHG emissions

Figure 6.18 shows that reduction of total GHG emissions by improved wastage flow rate selection in the DCL control strategy is likely to be undesirable since, in addition to increasing the EQI (i.e. reducing the effluent quality, as discussed in Section 6.2.4), it increases GHG emissions that would be reported under the CRC, thereby increasing the number of carbon credits that must be purchased and providing a financial deterrent.

Solutions providing the greatest reduction in total GHG emissions (such as solution A) also result in a reduction of energy related emissions, but to a lesser degree. Those which give a large reduction in total GHG emissions whilst retaining a high effluent quality (such as solution B) offer comparatively little improvement in GHG emissions associated with energy use, again suggesting that design of control strategies simply to reduce emissions reported under the CRC will hinder progress in cutting total GHG emissions.

6.3.3 Conclusions

The fact that solutions exist which provide a substantial reduction in total GHG emissions whilst maintaining a very good effluent quality but actually result in an increase in emissions associated with energy use suggests that attempting to reduce only emissions reported under the CRC is not the best approach to mitigating the effects of global warming. The results of this study demonstrate that, in some instances, an increase in energy use may be desirable if the net result is a reduction in emissions, yet the CRC acts as a deterrent to implementation of such solutions in the UK.

7 INVESTIGATING THE IMPACT OF CONTROL STRATEGY OPTIMISATION TO REDUCE GREENHOUSE GAS EMISSIONS ON RELIABILITY, ROBUSTNESS AND RESILIENCE

7.1 Introduction

Performance of dynamic systems is commonly measured using indicators such as the mean and/or variance of system outputs. However, whilst these are useful statistics, they are insufficient to describe how poorly the system will perform in the case of a failure and do not indicate how frequent or severe periods of poor performance may be (Hashimoto et al. 1982b); ideally, systems should be designed so that they rapidly recover and return to a satisfactory state following failure. Furthermore, the design of a system is based on forecasted or assumed conditions (such as service demand, flow rates, influent pollutant loads and costs), taking into account their impact on relevant constraints and environmental impacts. If these predicted conditions are inaccurate, the originally proposed project design may perform worse than another design which is better suited to the actual conditions.

In this research, WWTP control strategies have been optimised using modelled performance under pre-defined scenarios. In reality, however, there are many sources of uncertainties – including in the WWTP modelling and in the real-life conditions. Furthermore, since the optimisation problem is static, performance modelled during objective function evaluation is only valid for a limited time due to the dynamic nature of reality: external conditions change and environmental parameters fluctuate, plant equipment will deteriorate, and parts of the system may be replaced (Beyer and Sendhoff 2007). Classical optimisation procedures to identify the lowest cost solution meeting specified performance criteria and constraints might select a solution which tolerates system perturbations poorly (Fiering 1982). There are infinite possible scenarios that could occur – clearly these cannot all be analysed, and a single set of solutions that is optimal under every possible future, accounting for every uncertainty, cannot be developed – however, through analysis of reliability, robustness and resilience, preferable solutions can be identified, taking into account their performance under design conditions, response to uncertainties and their recovery from failures.

Reliability can be defined as “*The ability of a product, etc., to perform in a required manner, or produce a desired result consistently*” (Oxford English Dictionary 2010a). In an engineering context, reliability is a widely used performance criterion and provides a measure of system performance under design conditions, based on the probability or frequency of being in a non-failure state (Hashimoto et al. 1982b). A reliable solution will, therefore, minimise failure frequency under standard loading.

A wide range of definitions have been proposed for robustness (e.g. Hashimoto et al. 1982a, Deb and Gupta 2006, Lempert et al. 2006) and resilience (e.g. Holling 1973, Hashimoto et al. 1982b) for different scenarios and applications. The dictionary definition for ‘robustness’ is: “*The condition or quality of being robust (in various senses); sturdiness, hardiness; strength*” (Oxford English Dictionary 2010d), where relevant definitions of robust include “*yielding approximately correct results despite the falsity of certain assumptions underlying it... largely independent of certain aspects of the input*” and “*of a program: able to recover from errors; unlikely to fail, reliable*” (Oxford English Dictionary 2010c). Resilience is defined as: “*The quality or fact of being able to recover quickly or easily from, or resist being affected by a misfortune, shock, illness etc.; robustness; adaptability*” (Oxford English Dictionary 2010b). In essence, a robust solution will perform well across a wide range of possible scenarios when compared with the alternatives, considering the numerous sources of uncertainty in the model predictions. Robustness is a component of resilience (Bruneau and Reinhorn 2006), and in addition to being robust, a resilient solution is expected to resist and/or recover quickly from the effects of an unexpected event.

Simulation of WWTPs can be a useful tool for development of efficient and innovative operational control strategies. If these are to be successful in reality, they must also be reliable and robust (Rosen et al. 2008), since unexpected events (such as faults and failures and changing conditions) not considered in the modelling and evaluation can be detrimental to performance. Long term performance evaluation of the control strategies optimised based on their performance over two one-week periods, for example, shows that a significant proportion fail to maintain legislative compliance – highlighting the importance of considering further performance measures during the strategy selection.

It is debatable whether or not the concept of resilience can be applied to control strategies, since Holling (1973) stated that resilience is a property of a system; this would imply that the system in which the control strategy operates may be resilient, but not the control strategy itself. However, this original definition referred to 'ecological resilience', and the concept has since been applied in other spheres, including 'socio-ecological resilience', 'socio-technical resilience', 'engineering resilience', 'infrastructure system resilience' and 'institutional or organisational resilience' (e.g. Gallopin 2006, Blockley et al. 2012, Francis and Bekera 2014), and adapted accordingly. Holling (1973) also stated that resilience concerns the probability of extinction, which in the context of control strategies might be interpreted as the probability that the system does not recover from a failure. Adaptive capacity may also be considered a component of resilience (Francis and Bekera 2014), which suggests control strategies may be modified to aid recovery following failure – adding to the notion that it is the system that has resilience rather than the control strategy. In the case of long term gradual changes, such as population increase, it is plain that a change in control would be implemented to maintain a sufficient level of service. However, the system may be expected to recover from other disturbances which cause a reduction in performance, such as intermittent sensor failure, without control intervention; in such cases the concept of resilience is relevant.

It is particularly important to consider robustness and resilience when carrying out optimisation, since performance evaluation is based on models. These only represent an approximation of reality and, without detailed knowledge of the error function of the model, it is not known for certain whether the modelled optimum is also the true optimum (Beyer and Sendhoff 2007). The effects of inherent model uncertainty and unpredicted external disturbances are both important considerations (Logist et al. 2011).

Uncertainty in decision variable values when implementing an optimised solution (i.e. when a solution cannot be implemented with a sufficiently high degree of precision) will have a significant impact on system performance if the solution is sensitive to variable perturbations. This means that a global optimum solution may not be the best solution if objective values in practice differ from the theoretical ones. To be robust, therefore, optimal solutions must

demonstrate insensitivity to small perturbations in their decision variable values (Deb and Gupta 2005).

Development of more robust solutions typically corresponds with a reduction in performance (Logist et al. 2011), so maximising robustness can be viewed as an additional, conflicting objective in optimisation problems. 'Robust optimisation' can be used to account for model uncertainties and ensure that critical constraints will be met; however this requires multiple objective function evaluations for each solution (Deb and Gupta 2006), and therefore significantly increases the computational demand. Multi-objective optimisation using dynamic WWTP simulations is already very computationally demanding, even when just considering standard performance indicators/objectives and carrying out one performance evaluation for each solution, and robust optimisation techniques would be prohibitively expensive.

This study, therefore, aims to investigate the reliability, robustness and resilience of optimised control strategies (rather than optimise to maximise reliability, robustness and resilience), and identify previously un-explored relationships between control strategy design, performance (in terms of GHG emissions, operational costs and effluent quality), reliability, robustness and resilience. Optimised control strategies are also compared with the base case control strategy to identify possible effects of optimisation to improve GHG emissions, operational costs and effluent quality on reliability, robustness and resilience. In this research, reliability is evaluated based on the UWWTD requirements and performance over a one-year period with a single pre-defined design load. The robustness and resilience of optimised control strategies are assessed with regard to specific threats. It is impossible to consider every possible scenario which might impact upon performance, so in this instance two examples have been selected. This enables identification of solutions which perform better with regard to these specific issues and is illustrative of the proposed assessment methodology. However, performance in terms of robustness and resilience to other threats will clearly differ, so it is not possible to make a generic claim based on these results that a particular control strategy is 'most robust' or 'most resilient' – further investigation should be carried out if knowledge of the response to other threats or uncertainties is required.

7.2 Defining Reliability, Resilience and Robustness

7.2.1 Review

Reliability

Reliability is well defined, and typically taken to be a measure of the frequency or probability that a system achieves satisfactory performance (Hashimoto et al. 1982b, Maier et al. 2001, Kjeldsen and Rosbjerg 2004). It may also be stated that reliability relates only to performance under specified or design conditions and for a specified period of time (e.g. Niku et al. 1979).

In the context of WWTP performance, reliability is equivalent to the percentage of time in which effluent quality is expected to comply with specified discharge standards (Oliveira and Von Sperling 2008). Alternatively, reliability may be expressed as the proportion of time in non-failure state, using Eq. 7.1 (Kjeldsen and Rosbjerg 2004); this is based on occurrence of recorded failures rather than the probability of predicted failures.

$$\text{Reliability} = 1 - \frac{\sum_{k=1}^M F_k}{N} \quad \text{Eq. 7.1}$$

where:

F_k = Duration (number of time steps) of k th failure event

M = Number of failure events

N = Total number of time steps

If no failures occur within the design period, then the plant is completely reliable. However, due to uncertainties in the design and operation of WWTPs, failure risk is unavoidable and an acceptable level of risk should be specified (Oliveira and Von Sperling 2008). This is reflected in the 95 percentile limits set under the UWWTD.

Niku et al. (1979) proposed a coefficient of reliability (COR) (Eq. 7.2 and Eq. 7.3), using probability to relate required standard (X_S) to the mean effluent concentration (m_X). This is not a measure of reliability, however, but can be used to determine the design mean effluent concentrations required to meet a

given discharge standards with a specified reliability, provided the coefficient of variability is known.

$$m_x = (\text{COR})X_S \quad \text{Eq. 7.2}$$

$$\text{COR} = \sqrt{V^2 + 1} \times \exp(-Z_{1-\alpha}\sqrt{\ln(V^2 + 1)}) \quad \text{Eq. 7.3}$$

where:

V = Coefficient of variation

$Z_{1-\alpha}$ = Standardised normal variate (normal variate with a mean of zero and a standard deviation of one)

This has been implemented in analysis of WWTP performance with respect to different water quality parameters (Oliveira and Von Sperling 2008, Dong et al. 2012), using Eq. 7.4 and standard normal variate tables to determine the expected percentage compliance with specific discharge standards.

$$Z_{1-\alpha} = \frac{\ln X_S - (\ln m_x - 0.5 \ln(V^2 + 1))}{\sqrt{\ln(V^2 + 1)}} \quad \text{Eq. 7.4}$$

Robustness

Definitions of robustness provided in literature differ depending on the context and application, with some being very case specific. Hashimoto et al., for example, linked robustness explicitly to cost, stating that “*robustness describes the possible deviation between the actual costs of a proposed project and those of the least cost project design*” (Hashimoto et al. 1982b), and classified robust project designs and operating policies as those which are sufficiently flexible to allow their adaptation to a wide range of possible future conditions at little additional cost (Hashimoto et al. 1982a). Others are more generic and not restricted to the effects on a particular performance measure – for example, a robust solution can be taken as one in which the optimal design parameter values would remain unchanged if future demand conditions were to differ from those for which the project was designed (Fiering, 1976 and Matalas and Fiering, 1977 in (Hashimoto et al. 1982a)). Alternatively, a similar but less restrictive interpretation of a robust solution (in the context of control strategy design) is one which performs relatively well with respect to alternatives across

a wide range of plausible futures (Lempert et al. 2006). Definitions of robustness also differ between scientific fields. For example, Mens et al. (2011) distinguished between ‘system robustness’ and ‘decision robustness’, defining them as “*a system’s ability to remain functioning under disturbances*” and a representation of “*how sensitive a particular design is to uncertainties*” respectively. There is some overlap here with definitions of resilience, which typically concern the response of a system with regard to failures, but Jung et al. (2013) made clear that robustness does not include behaviour following failure, defining it as “*a system’s ability to stay within satisfactory bounds against variations in system factors*”.

Despite the wide range of definitions, however, all relate robustness to the impact of some type of uncertainty (whether in future conditions, the presence of future disturbances, decision variables or something else) on performance. Key to a robust solution is the ability to retain an acceptable level of functionality under uncertainties. Previous studies have considered robustness with regard to specific sets of uncertainties. For example, Deb and Gupta (2005) related the robustness of Pareto optimal solutions in multi-objective optimisation and the sensitivity of solution performance to uncertainty in implemented decision variable values, and Lempert et al. (2006) related robustness to performance under uncertain future scenarios.

There is no clear consensus on a suitable methodology for assessing robustness, and a wide range of methods have been used in previous studies. For example, Hashimoto et al. (1982a) suggest the use of a probabilistic robustness, using a defined probability density function for likely future demand to calculate the probability that the performance will remain within defined acceptable limits, whilst Mens et al. (2011) analysed the system response curve for change in uncertain parameters.

For assessment of optimised control strategy robustness, applying the robust solution definition of Fiering (Fiering, 1976 in (Hashimoto et al. 1982a)) (‘one in which the optimal design parameter values would remain unchanged if future demand conditions were to differ from those for which the project was designed’) would require the optimisation process to be repeated to identify optimum parameter values under each possible future. This is impractical in this study, a) due to the high computational demand of the optimisation process,

and b) due to the fact that the problem is multi-objective, hence a single optimum solution cannot be identified.

With regard to the impacts of uncertainty in decision variable values on the objectives in an optimisation problem, a robust solution can be defined as “one which is less sensitive to the perturbation of the decision variables in its neighbourhood” (Deb and Gupta 2006). For a single objective optimisation problem, minimise $f(x)$, with one decision variable (x), this concept can be shown in Figure 7.1. Solution B provides the minimum objective function value, but would not be recommended in practice as it is very sensitive to perturbations in the decision variable. Solution A, on the other hand, is considered a robust solution since the objective function value differs little with small variations in the decision variable. In a multi-objective problem, the sensitivity of each solution to perturbations in the decision variable values must be established with respect to each of the objectives.

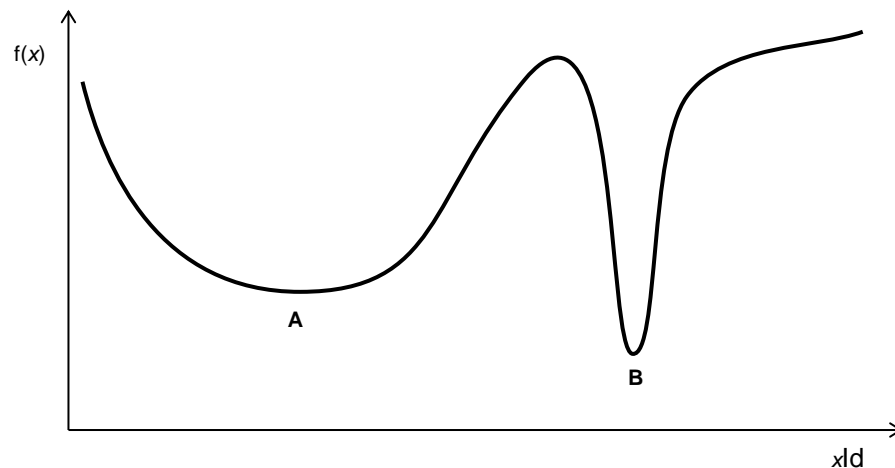


Figure 7.1: Illustration of global optimum and robust solutions in a single objective minimisation problem (adapted from Deb and Gupta 2006)

The decision variable, x , shown in Figure 7.1 could be replaced with any uncertain parameter and the visual representation of a robust and less robust solution would remain valid. This explanation of the concept of robustness does not provide a means by which it can be measured, however, a number of indicators have been proposed. In the context of BSM1, Vanrolleghem and Gillot (2002) defined a robustness index to provide a measure of the extent to which a control strategy continues to give good results under differing plant

conditions, based on the results of a GSA: relative sensitivity indices are calculated for uncertain plant parameters and these are then combined to give a single measure of global sensitivity (for a particular output), the inverse of which is used to quantify robustness. Whilst this method is useful in that it provides a single robustness index for each model output, taking into account multiple sources of uncertainty, it has the disadvantage of requiring a full GSA for each control strategy under evaluation, which would be prohibitively computationally demanding in this study. It also does not provide any information on the extent to which the performance is affected by any specific uncertainty, and does not take into account safety margins (or differences between the standard and minimum acceptable levels of performance) and the fact that limited variation in particular outputs may be completely acceptable.

Mens et al. (2011) provided an alternative representation and set of indicators for robustness, based on a theoretical system response curve (shown in Figure 7.2). As they defined robustness as “*a system’s ability to remain functioning under disturbances*”, suggested indicators therefore describe the response of the system up to the point from which it can no longer recover.

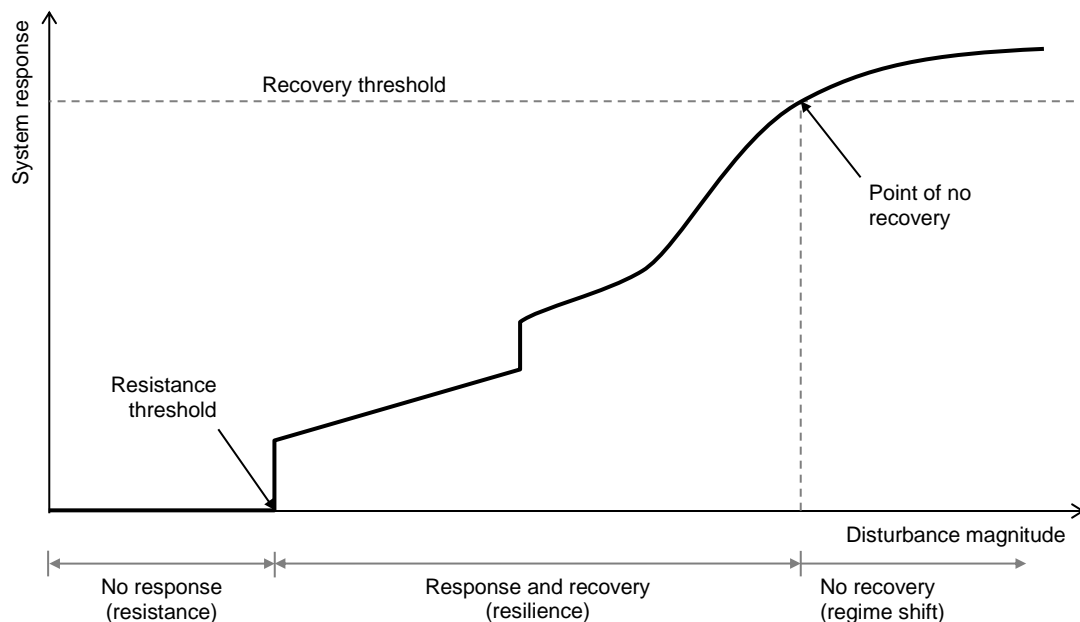


Figure 7.2: Theoretical response curve, identifying resistance, resilience, point of regime shift and recovery threshold (Mens et al. 2011)

Four robustness indicators are used to provide a comprehensive description of the response curve shown in Figure 7.2:

1. Resistance threshold – *The maximum disturbance magnitude for which there is negligible system response.*
2. Response severity – *A measure of the impact of disturbances over a range of magnitudes, which may be calculated as the area under the response curve.*
3. Proportionality of the response / Graduality – *A measure of the change in response with respect to change in disturbance magnitude, calculated using Eq. 7.5. This may be applied to the entire response curve or up to a defined disturbance magnitude.*

$$G = 1 - \frac{1}{2} \sum_{n=1}^N \left| \frac{\Delta D_n}{D_{max} - D_{min}} - \frac{\Delta R_n}{R_{max} - R_{min}} \right| \quad \text{Eq. 7.5}$$

where

- G = Graduality (-)
- ΔD_n = Change in disturbance for section n ($D_n - D_{n-1}$)
- ΔR_n = Change in response for section n ($R_n - R_{n-1}$)
- R_{max} = Response at point of no recovery
- D_{max} = Disturbance magnitude that corresponds to R_{max}
- D_{min} = Minimum disturbance magnitude
- R_{min} = Response corresponding to D_{min}
- N = Total number of sections

4. Point of no recovery – *The point (or area, if there is not a distinct point) at which the recovery threshold is crossed.*

These indicators do not take into account the effects of interactions between any of the uncertain parameters, only providing a measure of the robustness of one specific performance indicator to one specific source of uncertainty, but they do provide a detailed description of the system response and enable comparison of the effects of different sources of uncertainty.

This visual representation of robustness, which includes a region of system response labelled 'resilience', contradicts suggestion that robustness is a component of resilience (Bruneau and Reinhorn 2006). It also does not include identification of a failure point, beyond which performance is unacceptable – although in the context of flooding (as considered by Mens et al. (2011)), this may be equivalent to the resistance threshold, since any event which exceeds the flood protection level may be deemed a failure. For a different system, therefore, the system response at failure point would not be zero and response severity could be calculated based on behaviour in this region. It could also be argued that the 'graduality' is a component of resilience (De Bruijn 2004) rather than robustness.

Resilience

As for robustness, several definitions have been suggested for resilience. Hashimoto et al. (1982b), for example, described resilience as a measure of how quickly a system returns to a satisfactory state (i.e. recovers) following the occurrence of a failure. This differs somewhat from the definition of Holling (1973), who differentiates between resilience and stability: stability is the "*ability of a system to return to an equilibrium state after a temporary disturbance*" and a more rapid return with less fluctuation equates to a more stable system, whereas resilience is defined as a measure of the ability of a system "*to absorb changes of state variables, driving variables and parameters and still persist*". Systems with a low stability may be highly resilient due to a high capacity to absorb extremes of fluctuation (Holling 1973). Entering failure state is not involved in this definition of Holling (1973), although in the context in which it was applied (ecosystems) it may not be relevant due to different use of the terminology (i.e. a complete failure in an ecological sense might correspond to the ecosystem being destroyed, from which there can be no recovery, but in an engineering sense might correspond with an unacceptable drop in performance which can be rectified).

The ability of and speed by which a system recovers following failure are common themes in definitions of resilience, and resilience has been described as:

- “*The ability of the system to return to non-failure state after a failure has occurred*” (Kjeldsen and Rosbjerg 2004).
- A measure of the recovery capacity of a system from a state of failure to a functional state, where the main failure mode from which a system is capable of recovering is performance failure (Li and Lence 2007).
- The probability that a system recovers in the following moment given that the system is in failure state (Loucks 1997, Li and Lence 2007).

These definitions focus solely on the recovery of a system to a non-failure state following failure, without taking into account the probability of failure or behaviour of the system before and after entering failure state. In contrast, Bruneau et al. (2003) considered behaviour of the system within its acceptable operational mode (i.e. reliability) as well as when it is in failure state components of resilience, suggesting that resilient infrastructure exhibits a low probability of failure, low consequences of failure and low time to recovery. If it is accepted that robustness is necessary for resilience (Blockley et al. 2012), the definition for resilience cannot only include behaviour whilst the system is in failure state, since robustness relates to system response within the acceptable limit.

System response to a shock event can be described in terms of its amplitude, graduality and recovery rate. To comprehensively quantify resilience, indicators are required for all three of these aspects (De Bruijn 2004). It has been suggested that resilience can be calculated as the average probability that a system recovers at time step $t + 1$, given that it is in a state of failure at time step t (Hashimoto et al. 1982b, Loucks 1997, Li and Lence 2007). This definition, however, only addresses the rapidity at which the system returns to a satisfactory state following failure, without accounting for the likelihood of a failure occurring or the amplitude or graduality of the response when it does.

Wang and Blackmore (2009) suggested that resilience is a “*family of ideas, not a single thing*” and consists of multiple aspects: ‘resilience against crossing a performance threshold’, ‘resilience for system response and recovery after negative impacts’ and ‘resilience for adaptive capacity and management’. ‘Resilience against crossing a performance threshold’ concerns small and large disturbances and is defined as the magnitude of disturbance that can be

absorbed by the system without it entering an alternative state (i.e. failure). In the context of a water resource system, the following indicator for resilience against crossing a performance threshold (R_V) has been proposed (Wang and Blackmore 2009):

$$R_V = \sum_{i=1}^N Y_i / \sum_{i=1}^N D_i \quad \text{Eq. 7.6}$$

Where

N = Number of time steps

Y_i = Supply at time step i

D_i = Demand at time step i

This takes into account both the magnitude and duration of performance failures, although is unable to differentiate between failures of low magnitude/long duration and those of high magnitude/short duration.

‘Resilience for response and recovery’ relates to the rate at which the system recovers following disturbances, and concentrates on the effects of low frequency, high-consequence disturbances. Indicators are based on either the mean time in failure state (Hashimoto et al. 1982b) (R_{T1} , Eq. 7.7) or the maximum time in failure state (Kjeldsen and Rosbjerg 2004) (R_{T2} , Eq. 7.8):

$$R_{T1} = \frac{N_e}{\sum_{k=1}^{N_e} F_k} \quad \text{Eq. 7.7}$$

$$R_{T2} = \frac{1}{\max_{k=1 \dots N_e} (F_k)} \quad \text{Eq. 7.8}$$

Where

N_e = Number of times failure state is entered

k = Failure number

F_k = Duration of failure event k

It has been suggested that the definition based on the maximum time in failure (R_{T2}) is best, since the mean failure duration may be affected by the presence

of short, insignificant events (Kundzewicz and Kindler 1995), but also argued that this may lead to selection of less desirable solutions in some situations (Srinivasan et al. 1999).

‘Resilience for adaptive capacity and management’ addresses the need for proactive monitoring of operational and management procedures, to enable adjustments to be made when there is a drift towards unsafe performance. This includes the ability to predict and prevent future failures (through awareness of system response, speculation and learning from experience), the ability to adapt in the case of an adverse event in order to prevent further worsening of the situation, and the ability to recover quickly whilst minimising losses (Wang and Blackmore 2009).

7.2.2 Chosen Definitions and Measures

For the purposes of this study, the following general definitions for reliability, robustness and resilience are applied:

RELIABILITY *“Ability to minimise failure frequency under routine/design conditions”*

“Degree to which the system minimises level of service failure frequency over its design life when subject to standard loading” (Butler et al. 2014)

ROBUSTNESS Degree to which the system is able to maintain an acceptable level of service when subject to a given threat

RESILIENCE *“Degree to which the system minimises level of service failure magnitude and duration over its design life when subject to exceptional conditions” (Butler et al. 2014)*

In these definitions, ‘threat’ and ‘exceptional conditions’ can refer to a source of uncertainty (such as uncertainty in modelling parameters, uncertainty in external conditions or uncertainty in future conditions/events), thereby encompassing a range of alternative definitions and applications of the terms in which the effects of uncertainties is key (e.g. Deb and Gupta 2005, Logist et al. 2011). Threats can be classified based on both their origin (internal or external) and their

temporality of change (shock/acute or stress/chronic). Examples of potential threats, in the context of WWTP control strategies, are given in Table 7.1.

Table 7.1: Examples of threats to WWTP control strategies

Origin	Temporality of change	
	Shock (acute)	Stress (chronic)
Internal	<ul style="list-style-type: none"> • Controller failure • Sensor failure 	<ul style="list-style-type: none"> • Wear and tear • Sensor drift
External	<ul style="list-style-type: none"> • Storm event, resulting in temporarily increased flow to plant • Pollution incident, resulting in shock loading to plant 	<ul style="list-style-type: none"> • Population increase, resulting in increase in wastewater volume requiring treatment • Climate change

The chosen definition for resilience addresses the time dependency included in a wide range of alternative definitions (e.g. Hashimoto et al. 1982b, De Bruijn 2004, Li and Lence 2007), assuming that assessment of ‘ability’ takes into account the speed and mode by which an acceptable level of service is resumed.

When calculating robustness and resilience indicator values, it is necessary to define what the threats being considered are, and upon what performance indicators their impacts are being analysed – i.e. it is necessary to specify robustness/resilience of *what* to *what*. In the context of the above definitions, this means that for an indicator to be fully defined it should be described as:

“Robustness of (*specified level of service measure*) to (*specified threat*)”

OR

“Resilience of (*specified level of service measure*) to (*specified threat*)”

For example, Ward et al. (2013) investigated the robustness of reservoir performance to climate change, and Zeferino et al. (2012) assessed the robustness of wastewater system costs and water quality parameters to changes in river flow.

Visualisation of the concept of robustness is based on the work of Mens et al. (2011). Their calculation of robustness indicators considers the entire response

curve, however, including the section deemed to correspond with resilience. This contradicts the notion that robustness is a component of resilience (Bruneau and Reinhorn 2006) (rather than resilience a component of robustness). Identification of system response curve regions corresponding to robust and resilient behaviour is, therefore, modified to include a distinction between performance providing an acceptable level of service (which contributes to assessment of both robustness and resilience) and performance which is unacceptable but not beyond the point of no recovery (contributing to assessment of resilience only), as shown in Figure 7.3. The failure point is now defined as the point at which the system fails to provide satisfactory performance (as in Hashimoto et al. (1982b) and Kjeldsen and Rosbjerg (2004)), and the point of no recovery is the point at which the system is no longer able to return to an acceptable level of service.

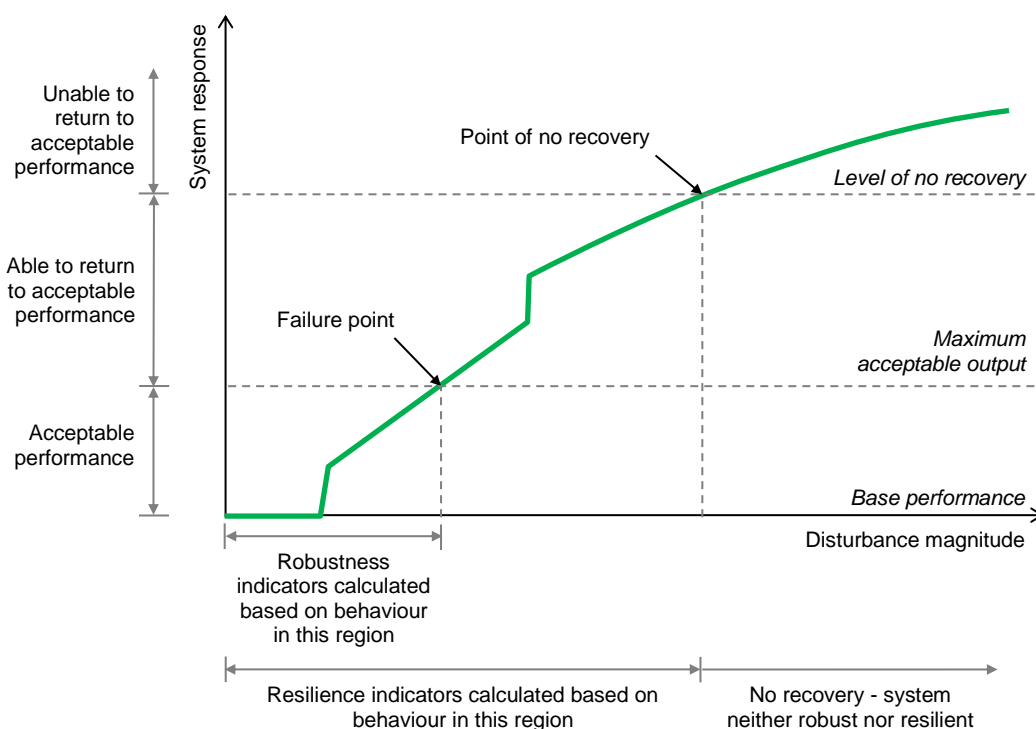


Figure 7.3: Visual representation of robustness and resilience components, based on system response with respect to disturbance magnitude

Whilst resilience concerns behaviour in the region indicated in Figure 7.3, resilience measures cannot be determined from this system response curve alone since knowledge of system response and recovery with respect to time is required. An example plot of system response as a function of time when

subject to disturbances (Figure 7.4) illustrates the components contributing to assessment of resilience.

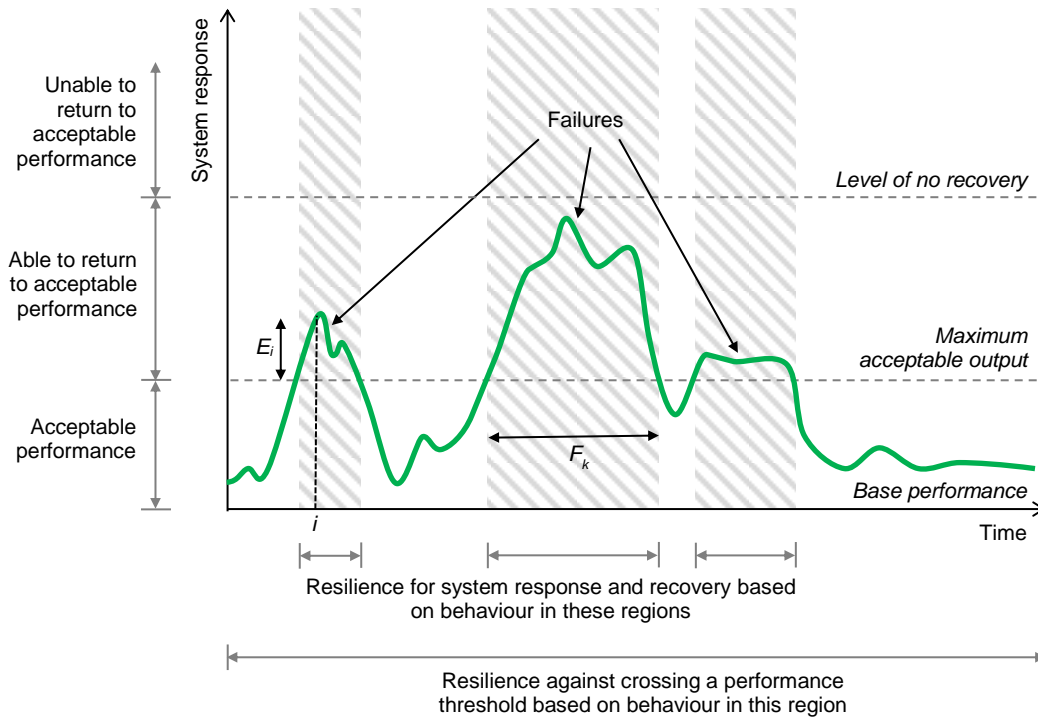


Figure 7.4: Visual representation of resilience components, based on system response with respect to time

Reliability Indicators

The proportion of time during which the system achieves acceptable performance when operating under design conditions, as detailed by Kjeldsen and Rosbjerg (2004), is the chosen measure for reliability. It is possible to calculate the expected percentage compliance based on the coefficient of variation of available data (using Eq. 7.4), but since sufficient data is available and it is not necessary to determine a new design standard that would be required to meet a specific level of reliability, it is more efficient to calculate reliability directly using Eq. 7.1.

Robustness Indicators

Robustness indicators are calculated from analysis of system responses to disturbances of different magnitudes, based on the methodology detailed by Mens et al. (2011) but using the modified response curve (system response as a function of disturbance magnitude) given in Figure 7.3.

The original response curve (Mens et al. 2011) (Figure 7.2) was proposed in the context of flood risk management, in which the region of no response corresponds to the flood protection level. This is not applicable in the context of WWTP control, however, where there is unlikely to be a disturbance magnitude that can be sustained with no notable system response (given that a large disturbance of that class does produce a response), so the robustness indicator 'response threshold' is not relevant in this case.

Response severity is calculated as the area under the response curve and provides a measure of the impact of disturbances over a range of magnitudes. In order to make the robustness indicators derived for different control strategies comparable, it is necessary to consider their responses over the same range of disturbance magnitudes – if area under the response curve up to the point at which failure occurs was calculated in each case instead, this could result in control strategies which reach failure at a very low disturbance magnitude receiving a low response severity whilst those which fail only under a much greater disturbance magnitude would receive a very high response severity. When disturbances of a specified maximum magnitude are applied, it is possible that the performance of some control strategies will exceed the acceptable limit (i.e. they will exhibit behaviour in the region of the response curve in Figure 7.3 corresponding to resilience only). In such instances the severity is still calculated based on the total area under the response curve, but the failure point must also be reported. Provided that the maximum disturbance magnitude applied is a realistic estimate of potential conditions, the response severity is of little relevance for any control strategy in which failure is observed during robustness analysis, since implementation would be inadvisable due to the high risk of failure.

Robustness indicators corresponding to instances in which the maximum acceptable system output is and is not exceeded under the specified maximum disturbance magnitude, and how these relate to the system response curve are shown in Figure 7.5a and Figure 7.5b respectively. In Figure 7.5a, the failure point is the normalised disturbance magnitude corresponding to the point at which the maximum acceptable output is exceeded, whereas in Figure 7.5b there is no failure point as acceptable performance is maintained under the

maximum disturbance. In both cases the response severity is equal to the total area under the response curve.

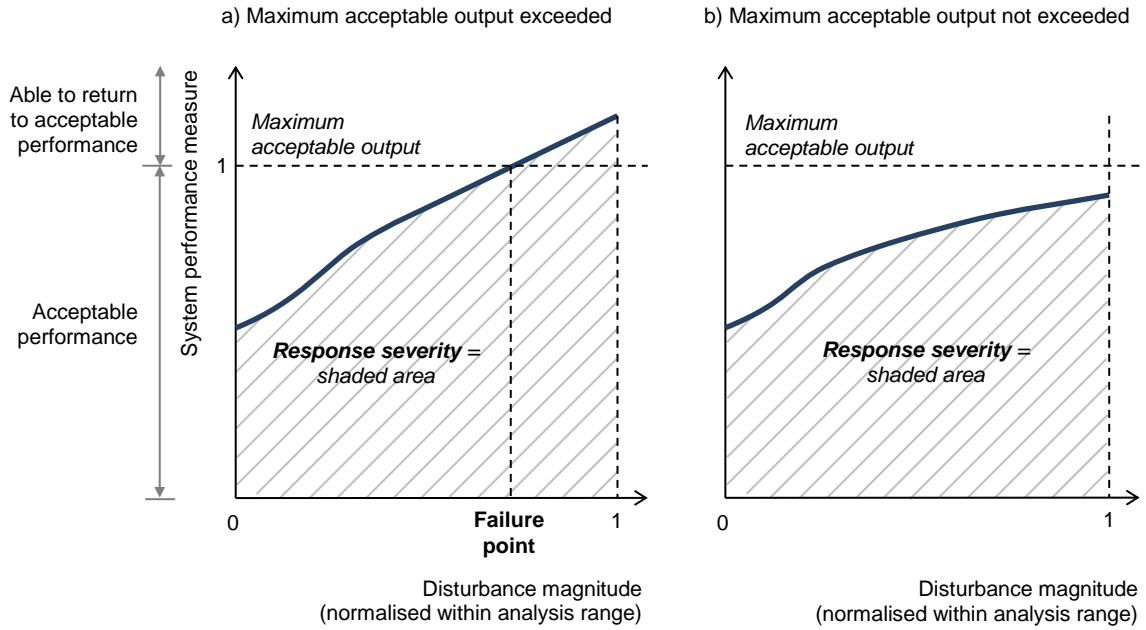


Figure 7.5: Robustness indicator components (shown in bold type) for instances in which the maximum acceptable system output is: a) exceeded, and b) not exceeded, under disturbances of a specified maximum magnitude

Resilience Indicators

In this study, resilience is assessed using the results of dynamic performance evaluation, based upon an adaptation of the method detailed by Wang and Blackmore (2009). Monte-Carlo simulation is used for assessment of dynamic performance, where multiple time series incorporating the uncertain conditions to which resilience is being assessed are evaluated. For each time series, resilience against crossing a performance threshold (R_V) and resilience for system response and recovery (R_{T1} and R_{T2}) are calculated. Calculation of R_{T1} and R_{T2} is unchanged from that of Wang and Blackmore (2009) – i.e. using Eq. 7.7 and Eq. 7.8. Calculation of R_V is carried out using Eq. 7.9, adapted from Eq. 7.6 (Wang and Blackmore 2009); in this application, $(T_i - E_i)$ replaces the model output at each time step, to account for instances in which the system output is greater than the required output value (which cannot occur in the original example, since the system supply cannot exceed the demand).

$$R_V = \frac{\sum_{i=1}^N (T_i - E_i)}{\sum_{i=1}^N T_i} \quad \text{Eq. 7.9}$$

where:

N = Number of time steps

T_i = Threshold (maximum acceptable output) at time step i

E_i = Exceedance at time step i

A visual representation of the dynamic response components contributing to resilience indicators R_V , R_{T1} and R_{T2} is given in Figure 7.4. Note that although the maximum acceptable output threshold shown takes a fixed value throughout the evaluation duration, a dynamic limit may be applied.

Wang and Blackmore (2009) calculated ‘average’ (presumably mean) values for each resilience indicator, based on Monte-Carlo simulation results, to enable comparison of different solutions. If there are any samples in which no failures occur, however, their R_{T1} and R_{T2} values will be infinite and consequently the indicator values for the solution will also be infinite. Therefore, it is proposed that median values are used to establish overall resilience indicators for each solution, based on their performance in each of the Monte-Carlo samples.

7.3 Reliability of Optimised Control Strategies

7.3.1 Reliability Assessment Methodology

Selection of Solutions for Analysis

Reliability is assessed for solutions derived using objective set Y (minimise EQI, OCI and GHG emissions) which better the base case GHG emissions whilst maintaining a compliant effluent. In order to reduce the number of solutions to a manageable level, the truncation method implemented in SPEA2 (Zitzler et al. 2001) is used to select 100 well-distributed solutions from the final generation. This is an iterative process in which the solution with the minimum distance to another solution is removed at each step.

Calculation of Reliability Measure

Reliability is a measure of system performance under design conditions and, in this study, it is assumed that these can be represented by the final 364 days of BSM2 dynamic influent data. To assess performance under these conditions, each solution is evaluated as detailed in Chapter 3, Section 3.5. This yields different results to the simulations carried out for control strategy optimisation, since these utilised two reduced evaluation periods, and solutions which achieved a compliant effluent quality during optimisation do not necessarily maintain this level of performance when evaluated over a longer period.

For each simulation, dynamic effluent BOD₅, COD, TSS and total nitrogen concentrations and rate of GHG emissions are recorded; reliability is then individually calculated for each performance indicator using Eq. 7.1. Failure limits for effluent quality components are based on the UWWTD requirements, and the 95th percentile value for dynamic GHG emissions under the base case solution is used for the GHG emission failure point (as summarised in Table 7.2).

Table 7.2: Failure points for reliability analysis

Performance measure	BOD ₅	COD	Total nitrogen	TSS	GHG emissions
Failure limit	25 g/m ³	125 g/m ³	15 g/m ³	35 g/m ³	1.22 kg CO ₂ e/m ³
Minimum reliability required to achieve UWWTD compliance	0.95	0.95	N/A	0.95	N/A

Given that the UWWTD requirements considered for BOD₅, COD and TSS are for 95 percentile concentrations rather than maximum concentrations, an exact failure point cannot be determined; if these are applied as absolute limits, however, a reliability of at least 0.95 will indicate compliance. For total nitrogen, the UWWTD specifies a maximum annual mean value, which cannot be translated to a minimum required reliability. For the purposes of reliability analysis, an absolute limit of 15 g N/m³ is specified, but it is important to note that full compliance can be maintained even if values in excess of this are reported and, as such, reliability indicators for total nitrogen are not expected to be as high as those for BOD₅, COD and TSS.

7.3.2 Reliability Assessment Results and Discussion

An overview of the reliability optimised solutions with respect to effluent quality requirements and GHG emissions is given in Figure 7.6. It is shown that all solutions achieve a BOD₅ reliability greater than 0.95 (i.e. they meet the UWWTD requirement), and at least 75% of solutions meet the COD and TSS requirements. For these indicators, the performance of optimised solutions is comparable with that of the base case. Effluent total nitrogen reliability, however, is significantly reduced by the optimisation process. This also differs considerably between solutions, with the best achieving a reliability of 1.00 and the worst a reliability of 0.00. A reliability of 1.00 is not necessarily required to achieve UWWTD compliance since the limit set for failure in reliability analysis is a mean performance criteria in reality, however, a reliability of 0.00 would certainly equate to non-compliance.

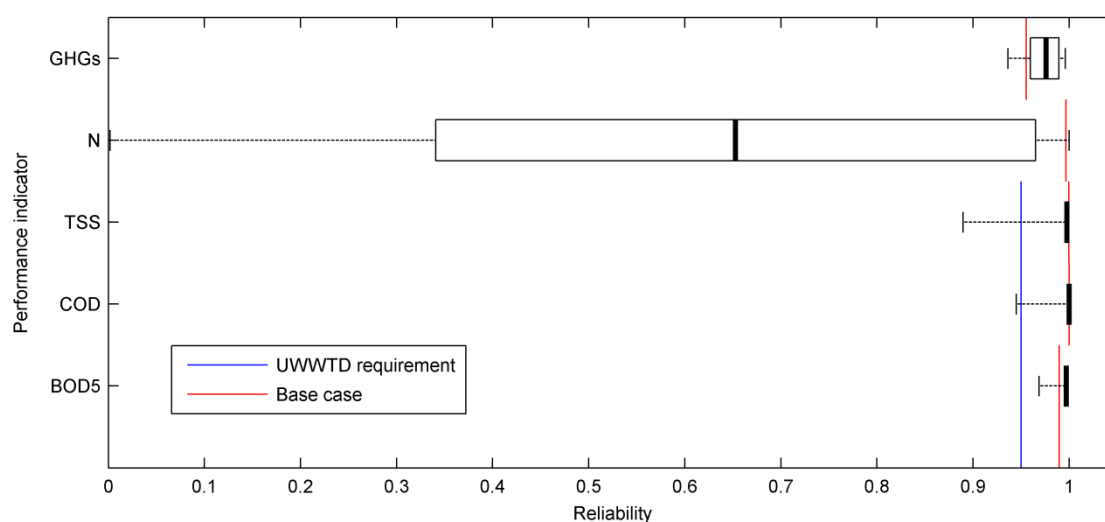


Figure 7.6: Overview of reliability indicators for 100 solutions analysed

Solutions are generally shown to perform favourably in terms of GHG emission reliability, with 94% achieving a 95 percentile less than that of the base case. This is predictable given that minimising GHG emissions was one of the optimisation objectives, but shows that multi-objective optimisation can successfully be used to generate solutions which reliably reduce emissions.

The minimum effluent quality reliability for each solution analysed is presented in Figure 7.7 (a complete set of reliability results with each performance indicator shown separately is provided in Appendix D). This figure includes identification of solutions deemed to have unacceptable effluent quality

reliability; for BOD₅, COD and TSS the limit is 0.95 (as required under the UWWTD), and for total nitrogen a reliability of less than 0.50 is considered insufficient. EQI, OCI and GHG emission values presented for each solution are those derived during control strategy optimisation, i.e. under a shortened evaluation period.

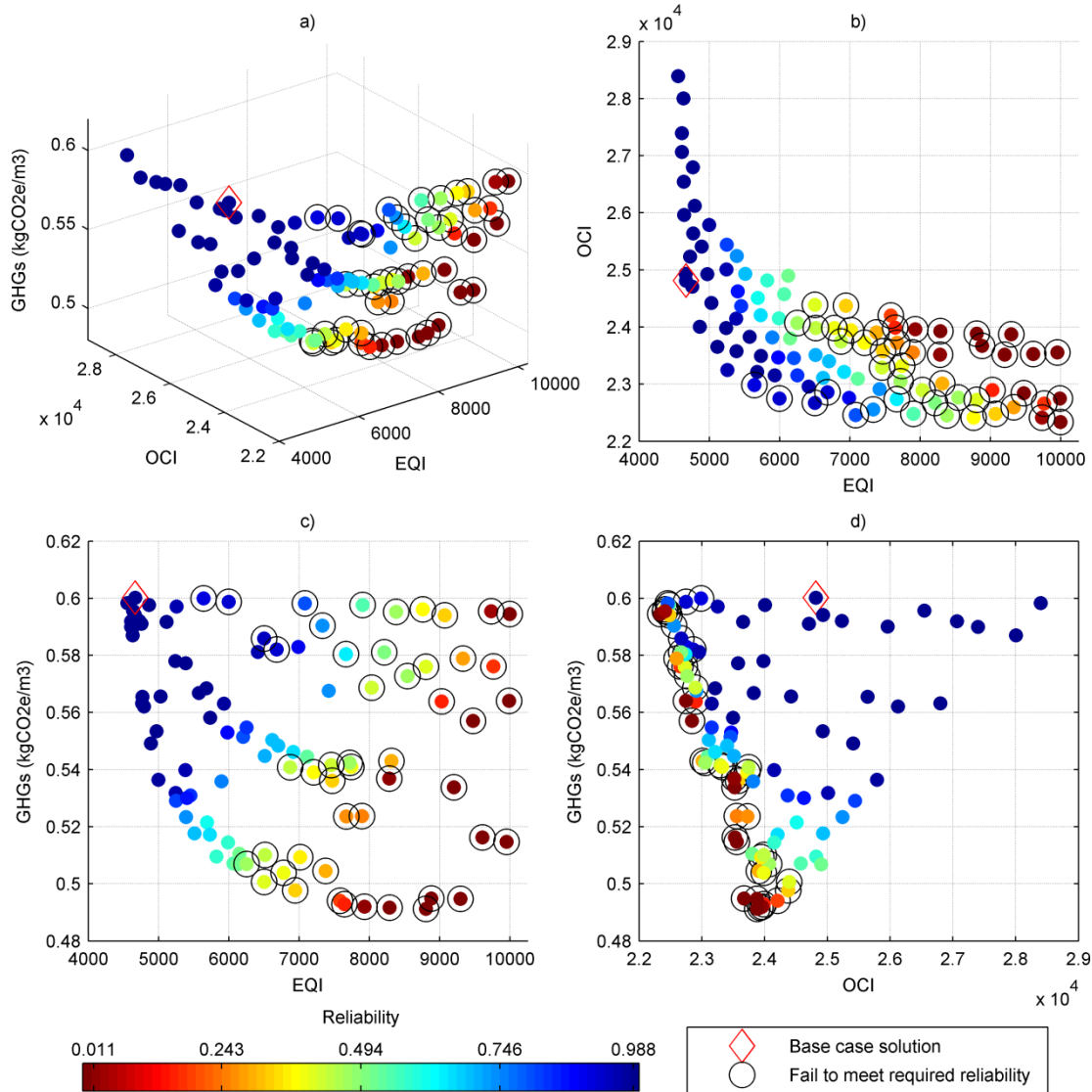


Figure 7.7: Minimum effluent quality reliability of non-dominated solutions bettering base case GHG emissions under default conditions, with solutions providing inadequate reliability identified

All solutions with an EQI greater than 7422 fail to meet the required effluent quality reliability standards, and there is a strong negative correlation between EQI and the effluent quality reliability ($r^2 = 0.79$). The most reliable solutions (in terms of effluent quality) are those with a low EQI and only a moderate reduction in GHG emissions. These are not the cheapest solutions, and Figure

7.7d shows that solutions which are optimal based on GHG emissions and OCI alone have unacceptable reliability.

The relationships between each individual reliability measure and the three performance indicators for which the solutions are optimised are presented in Figure 7.8. This shows that solutions with a high EQI predominantly fail due to unacceptable total nitrogen reliability, although TSS and COD reliability values below the UWWTD requirement are also observed. The lowest OCI solutions also have unacceptable effluent quality reliability (as shown in Figure 7.7), but where EQI is below 7422, this is due to COD and TSS failures rather than total nitrogen. This suggests that it may not be good practice to implement highly optimised solutions which appear to offer significant cost reductions whilst cutting GHG emissions based on the results of a short performance evaluation. If additional operational costs are acceptable then high effluent quality reliability can be achieved: all solutions with an OCI greater than 26,000 (representing a 4.8% increase from the base case) provide a total nitrogen reliability of 1.00 and a TSS and COD reliability greater than the UWWTD requirement. However, these solutions do not include those with the greatest emission reduction or greatest emission reduction reliability.

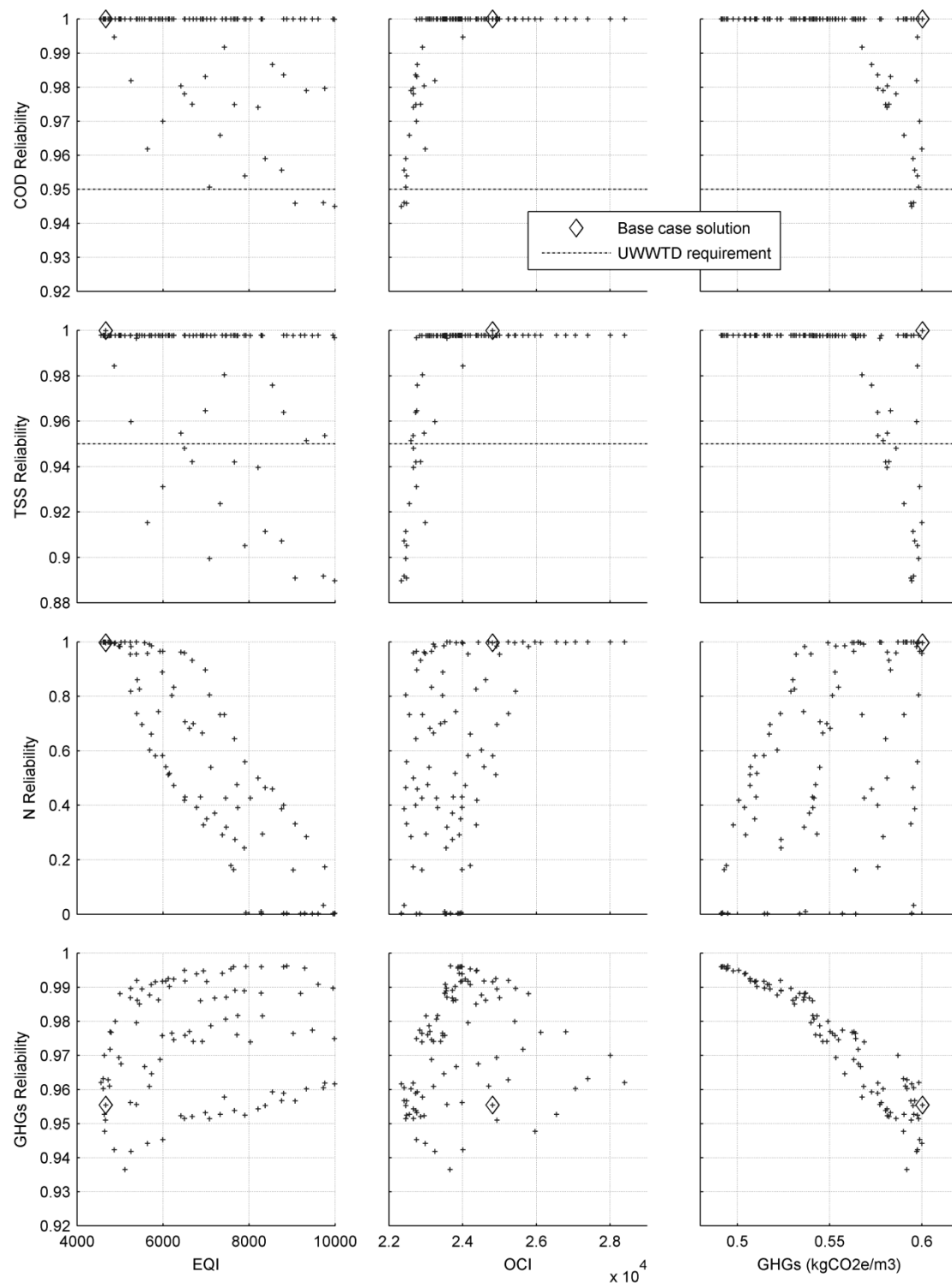


Figure 7.8: Relationship between reliability measures and performance indicators for non-dominated solutions bettering base case GHG emissions under default conditions

Comparison of decision variables and reliability measures of the optimised solutions, in order to identify characteristics which contribute to a reliable solution, shows few strong correlations (results summarised in Table 7.3).

Table 7.3: Correlation coefficients for relationships between decision variables and reliability measures; dark grey shading denotes strong correlation ($\bar{r} \geq 0.6$), light grey denotes moderate correlation ($0.4 \leq \bar{r} < 0.6$)

Variable	BOD ₅ reliability	COD reliability	TSS reliability	Total nitrogen reliability	GHGs reliability
Qintr (m ³ /d)	-0.05	-0.07	-0.07	-0.04	-0.03
Qw (m ³ /d)	0.74	0.76	0.77	-0.08	0.78
KLa1 (/d)	-0.33	-0.35	-0.35	-0.43	-0.12
KLa2 (/d)	-0.08	-0.10	-0.10	-0.45	-0.38
carb1 (m ³ /d)	0.17	0.21	0.21	0.38	-0.17
carb2 (m ³ /d)	0.26	0.27	0.28	0.03	0.32
carb5 (m ³ /d)	0.22	0.22	0.22	0.20	0.03
Controller setpoint (g/m ³)	0.31	0.34	0.34	0.59	-0.07
Controller offset	-0.13	-0.14	-0.14	-0.10	0.06
Controller amplification	-0.16	-0.20	-0.21	-0.01	-0.07
Controller integral time constant	0.08	0.06	0.06	-0.05	0.08
KLa3 gain	-0.17	-0.14	-0.14	-0.07	-0.31
KLa5 gain	-0.08	-0.10	-0.10	-0.06	-0.02

BOD₅, COD, TSS and GHG emission reliability all exhibit a strong positive correlation with wastage flow rate. The observed correlation between wastage flow rate and BOD₅, COD and TSS reliability appears somewhat counterintuitive, since an excessively low SRT (resulting from a high wastage flow rate) will prevent development of a stable population of bacteria and may result in washout (Grady et al. 1999), but a decrease in performance with respect to effluent COD and TSS at very high SRTs is not unexpected (e.g. Li and Wu 2014). These results are of little importance here, however, since BOD₅, COD and TSS reliability is not a major problem and 86% of solutions provide sufficient reliability for UWWTD compliance.

The GHG correlation suggests that design solutions with a high wastage flow rate may provide greater reliability in GHG emission reduction, but correlation does not imply causality. Optimised solutions which provide the greatest reduction in mean emissions typically utilise a high wastage flow rate (low SRT);

this corresponds with previous studies (Corominas et al. 2010, Ashrafi et al. 2014) in which a reduction in wastage flow rate (increase in SRT) in an aerobic treatment system was found to increase GHG emissions, yet it has been shown in Chapter 6, Section 6.2.4 and that emission reduction may also be achieved with low wastage flow (high SRT) rate solutions.

Moderate positive correlation between effluent total nitrogen reliability and the controller setpoint is also observed. Solutions which fail to meet the required reliability typically have a controller setpoint value of less than 0.64 g/m^3 , as shown in Figure 7.9a. Not all solutions with a setpoint of less than 0.64 g/m^3 have an unacceptable reliability, but a significantly greater proportion of solutions with a higher setpoint are acceptable (97% compared with 25%). This suggests that, in terms of reliability of nitrogen removal, a DO setpoint of at least 0.64 g/m^3 is preferable, but significant reduction with respect to the base case setpoint of 2 g/m^3 can be applied without compromising reliability. Such setpoints are at the lower end of the typical range of $0.5 - 2.0 \text{ g/m}^3$ (Wanner 1994), but it has been shown that complete nitrification can be achieved with a DO setpoint as low as 0.16 g/m^3 if the SRT is sufficiently long (Liu and Wang 2013). Figure 7.9b shows that restricting solutions to those with a setpoint greater than 0.64 g/m^3 would eliminate those providing the greatest GHG emission reduction, but still offer a wide range of solutions offering an emission reduction of up to 16%.

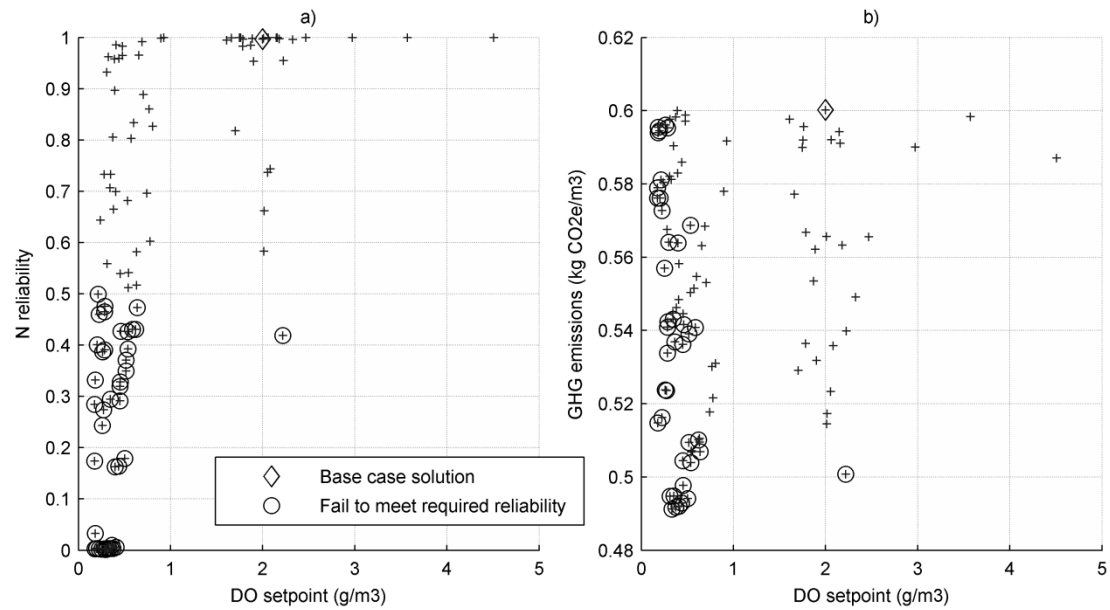


Figure 7.9: Relationship between decision variables and performance: a) DO setpoint and total nitrogen reliability; and b) DO setpoint and GHG emissions

Effluent total nitrogen reliability also exhibits a moderate negative correlation with KLa_1 and KLa_2 values, suggesting that low aeration intensities correspond with a more reliable solution. This is reflected in the fact that aeration is not conventionally applied in the first reactors of an activated sludge unit (which normally operate under anoxic conditions), and the impact of aeration on effluent nitrogen reliability is to be expected as it would create aerobic conditions and, therefore, reduce the denitrification efficiency.

7.4 Robustness of Optimised Control Strategies

7.4.1 Robustness Assessment Methodology

Robustness analysis is carried out for 100 solutions from the final (25th) optimisation generation which better base case GHG emissions whilst maintaining a compliant effluent when evaluated under default conditions, as for reliability. In order to determine whether less highly optimised solutions are more robust than those that are most highly optimised, robustness indicators are also calculated for non-dominated solutions from generations 10, 15 and 20. As for the final generation, these solution sets are each reduced to 100 well-distributed solutions using the truncation method implemented in SPEA2 (Zitzler et al. 2001).

Calculation of Robustness Measures

To calculate robustness indicators, it is necessary to derive response curves for each key model output with respect to each uncertain parameter under investigation. For each parameter, the response of effluent quality indicators used to assess UWWTD compliance (BOD₅, COD, total nitrogen and TSS) and of GHG emissions to influent disturbances is assessed. GHG emissions are measured in terms of kg CO₂e/d instead of kg CO₂e/m³, since one of the adjusted influent parameters is flow rate.

Selection of perturbations to which the WWTP is subjected is guided by previous calculation of robustness indices for control performance in the BSM1 (Vanrolleghem and Gillot 2002), in which uncertain characteristics include:

- a) Influent flow rate
- b) Influent total nitrogen concentration
- c) Influent COD concentration
- d) Temperature

Vanrolleghem and Gillot (2002) also investigated the effects of rain conditions and storm conditions (as the initial evaluation was under dry weather conditions) and of adjustment to the wastage flow rate (Q_w) and recycle flow rate (Q_r). However, since the BSM2 dynamic influent already incorporates dry weather, rain and storm conditions, and Q_w and Q_r are defined for each optimised solution, these are not included in this analysis.

To summarise, this study investigates the robustness of BOD₅, COD, total nitrogen, TSS and GHG emissions from optimised control strategy solutions to perturbations in influent flow rate, total nitrogen concentration, COD concentration and temperature.

Plant performance is evaluated under eleven different percentage magnitudes of change for each uncertain parameter, distributed evenly across the total range considered, to provide an estimation of each response curve. The magnitude of change allowed in each parameter is guided by the previous robustness study by Vanrolleghem and Gillot (2002), as summarised in Table 7.4. Model simulations are carried out as for the multi-objective optimisation (detailed in Chapter 6, Section 6.1.1), using two two-week periods – one winter

and one summer – with the final week of each used for evaluation. Effluent BOD₅, COD and TSS concentrations are reported as 95 percentile values whilst the annual mean value is given for total nitrogen, in accordance with the UWWTD compliance requirements.

Table 7.4: Uncertain parameters and range of percentage change used for robustness analysis

Parameter	Default mean value	Greatest change	Step size
Influent flow rate	20,648 m ³ /d	+ 10%	1%
Influent COD	592.5 g COD/m ³	- 10%	1%
Influent total nitrogen	66.2 g N/m ³	+10%	1%
Temperature	14.9°C	- 33.3%	3.33%

Robustness indicators detailed in Section 7.2.2 (response severity and failure point) are calculated as appropriate for each response curve. Response severity is calculated for every solution, disturbance type and output; the failure point is only calculated in instances where the maximum disturbance magnitude modelled is sufficient to cause failure. Breaching UWWTD effluent quality limits or the base case GHG emissions is considered a failure, and the failure point is determined using interpolation between known points on the response curve. Failure limits are summarised in Table 7.5.

Table 7.5: Failure points for robustness analysis

Performance measure	BOD ₅ 95 percentile	COD 95 percentile	Mean total nitrogen	TSS 95 percentile	Mean GHG emissions
Failure limit	25 g/m ³	125 g/m ³	15 g/m ³	35 g/m ³	24,046 kg CO ₂ e/d

To enable comparison of robustness indicators for different performance indicators and different classes of disturbance, disturbance magnitudes are normalised with respect to the maximum disturbance in each case and model outputs are normalised with respect to the acceptable range (i.e. from zero to the values given in Table 7.5). Therefore, all disturbance magnitudes are reported as values from 0-1 and model outputs which are compliant or better the base case fall in the range 0-1; outputs which exceed the acceptable limit (i.e. fail) take a value greater than one.

7.4.2 Robustness Assessment Results and Discussion

Response Severity and Failure Point

The severity of the most severe effluent quality response to any of the disturbances for each solution is shown in Figure 7.10, and the most severe response in terms of GHG emissions in Figure 7.11. In each figure, solutions for which at least one of the corresponding outputs reaches failure point under the given disturbance ranges are identified. Complete results, showing the severity of BOD₅, COD, total nitrogen, TSS and GHG emission responses to each of the four disturbances and any resultant failures individually, are provided in Appendix E. All solutions presented are compliant with the UWWTD, reduce the base case GHG emissions and are non-dominated based on EQI, OCI and GHG emissions when evaluated under default conditions.

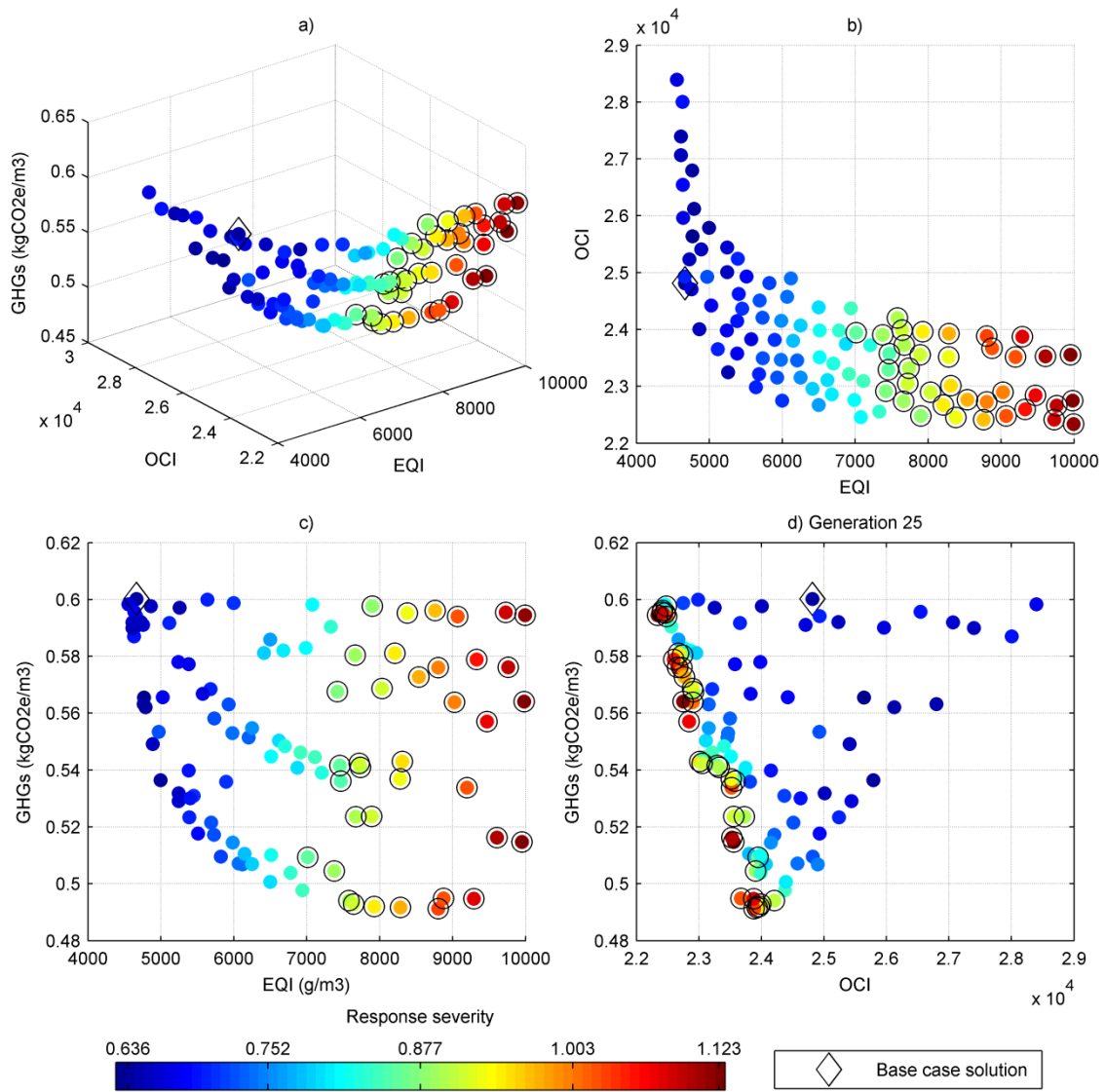


Figure 7.10: Worst case effluent quality response severities for non-dominated solutions which better the base case GHG emissions under default conditions, with solutions which reach failure point circled

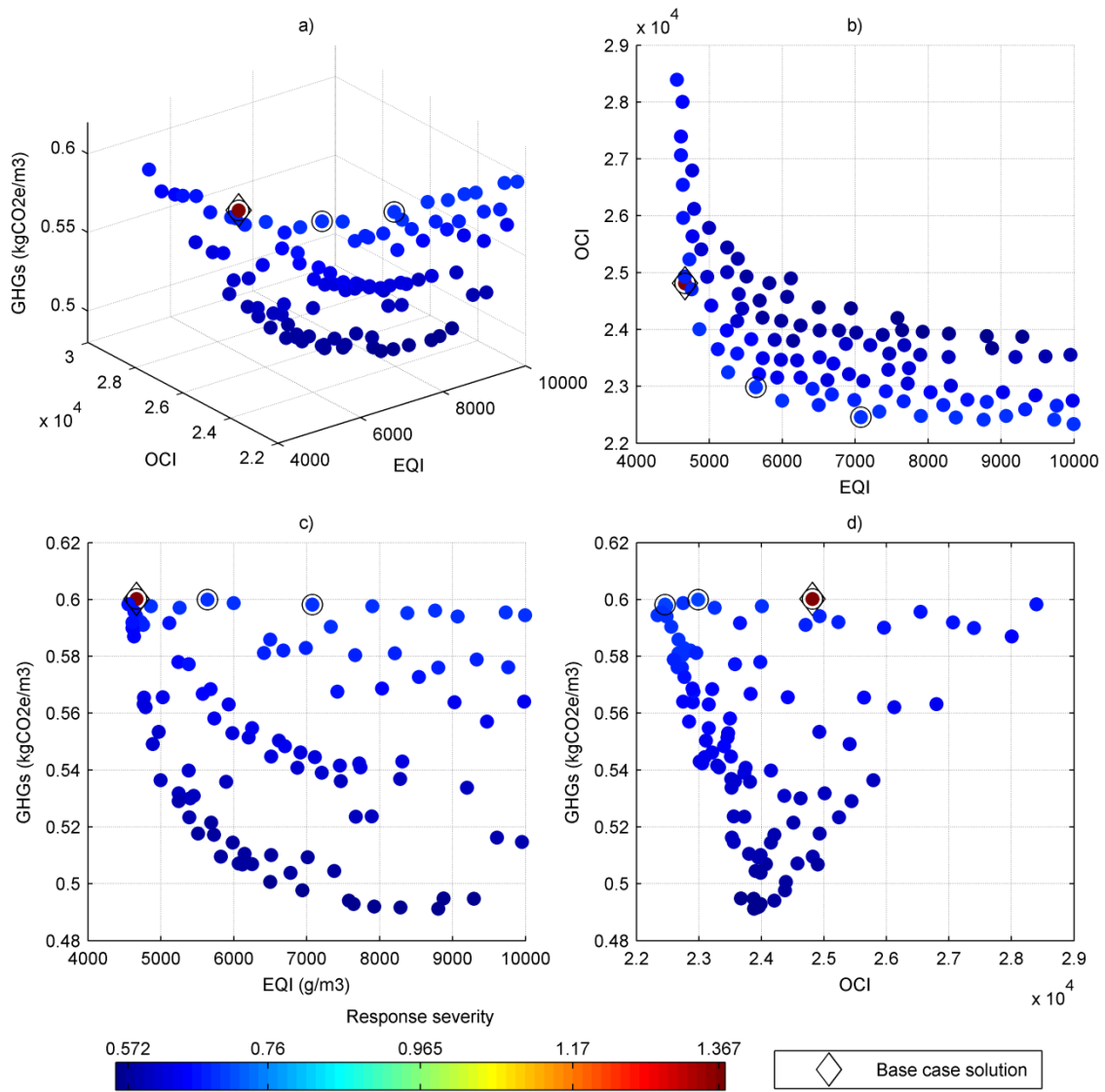


Figure 7.11: Worst case GHG emission response severities for non-dominated solutions which better the base case GHG emissions under default conditions, with solutions which reach failure point circled

Figure 7.10 shows that the highest EQI solutions have the highest effluent quality response severity and greatest occurrence of failure (predictably, since these provide an effluent closest to the failure limits under default conditions). All solutions with an EQI greater than 7330 fail to provide UWWTD compliance under the modelled disturbances and exhibit poor robustness. These high EQI solutions also correspond with those on the GHGs/OCI Pareto front, confirming that selection of control options on the basis of GHG emission and operational cost reduction alone, subject to achieving a compliant effluent under default conditions, is inadvisable. There is a very strong positive correlation between EQI and effluent quality response severity ($r = 0.99$), as shown in Figure 7.12,

and in order for solutions to be robust, they must provide an effluent quality significantly better than the compliance limit when operating under design conditions.

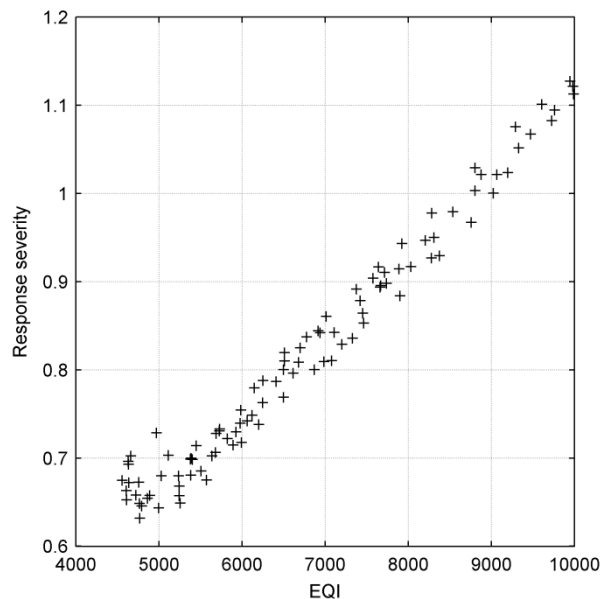


Figure 7.12: Relationship between EQI and worst case effluent quality response severity

All failures shown in Figure 7.10 result from exceedance of the mean effluent total nitrogen limit under one or more of the disturbances modelled; no failures in the BOD₅, COD or TSS responses are observed. Further detail on the type of disturbance which causes effluent nitrogen failure in each solution is given in Figure 7.13. All solutions which fail as a result of influent COD, flow rate or nitrogen disturbances also fail as a result of decreased temperature. This shows that, of the four disturbances considered, temperature poses the greatest threat and suggests that increasing robustness of effluent total nitrogen to temperature disturbance will have wider benefits in terms of overall robustness. This suggestion is supported somewhat by the previous finding that, under DO control, total costs (which include effluent fines) are most sensitive to a decrease in temperature (Vanrolleghem and Gillot 2002). The effects of combined disturbances may also be significant, and it has previously been found, for example, that high COD/N ratios destabilize the nitrification process particularly at low temperatures (Komorowska-Kaufman et al. 2006).

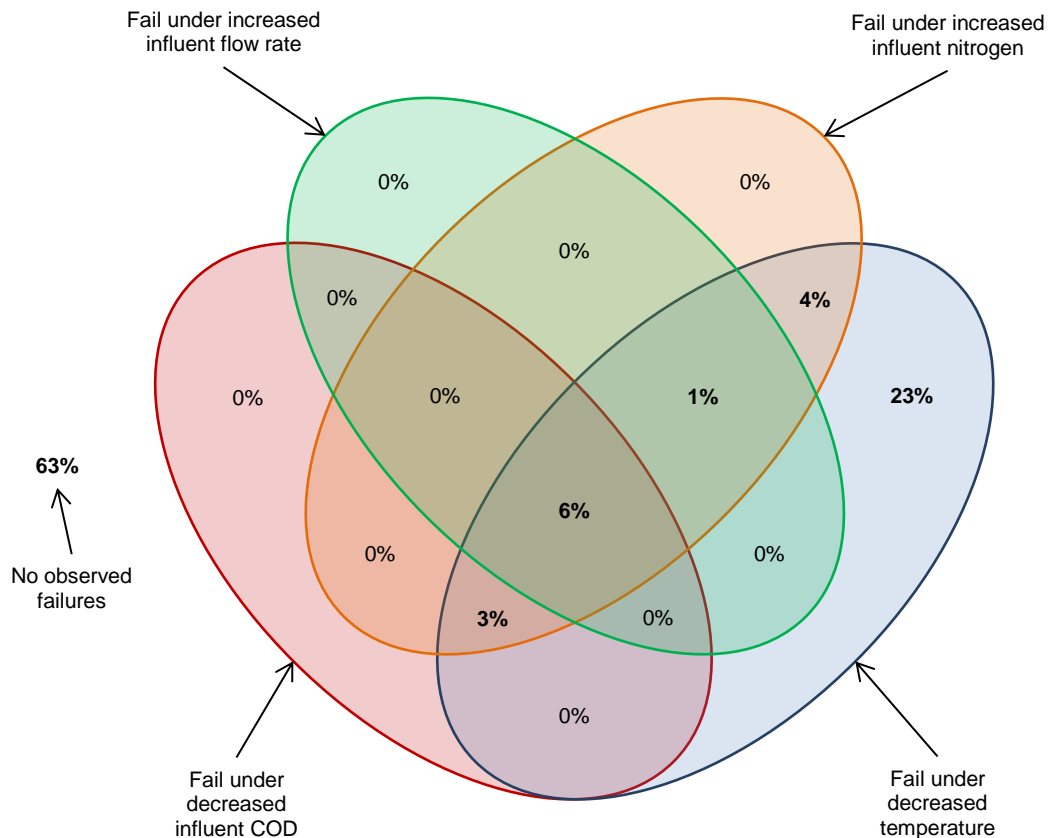


Figure 7.13: Venn diagram showing percentage of solutions which exceed effluent total nitrogen requirements under each disturbance

With respect to GHG emissions (Figure 7.11), only two optimised solutions reach failure point under the disturbance magnitudes considered; again, these result only from a decrease in temperature. Given that both these solutions provide negligible reduction in GHG emissions under normal operating conditions, however, their implementation would be undesirable regardless of their robustness. All solutions provide a significant reduction in response severity with respect to the base case.

Detailed Analysis of Select Solutions

Decision variable values and key performance indicators of solutions providing a reduction in GHG emissions of at least 10% with respect to the base case are presented in Figure 7.14, with response severity represented by a colour scale and solutions which reach failure point in robustness analysis shown in grey. Decision variables are normalised within the optimisation range; performance indicators and response severity are normalised from zero to the maximum

observed value. Response severities shown are the worst case effluent quality response severity for each solution.

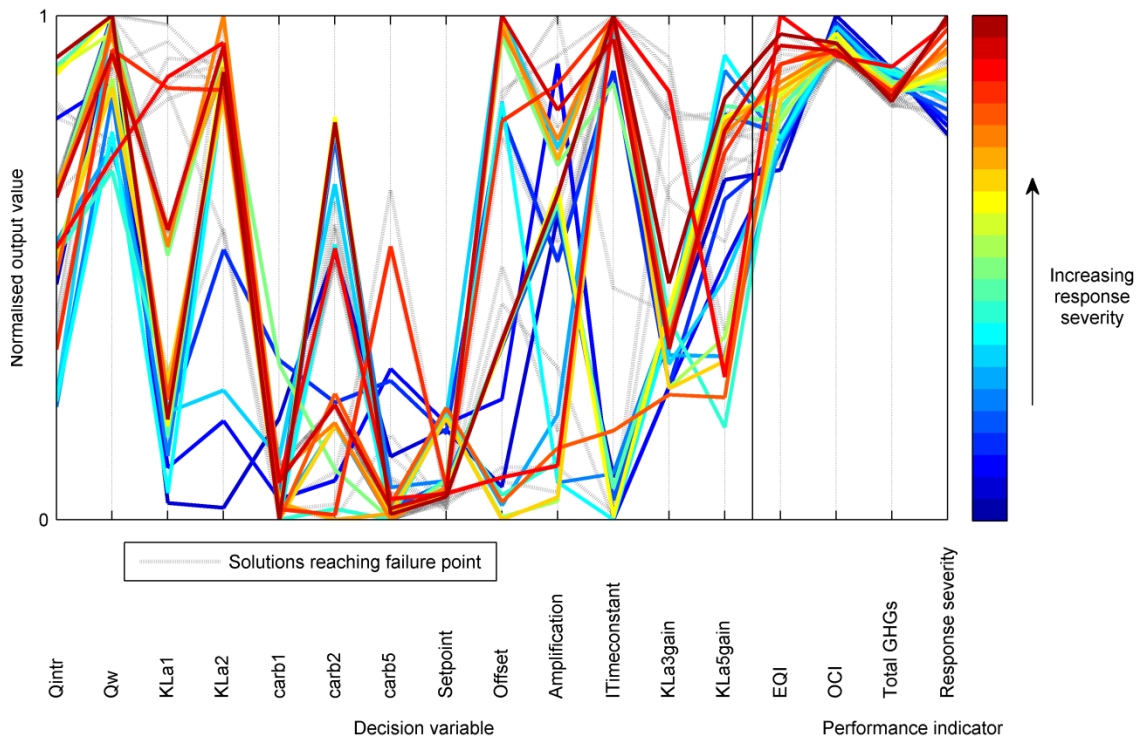


Figure 7.14: Decision variable values, key performance indicators and effluent quality robustness of solutions providing a reduction in GHG emissions of at least 10%

The most robust solutions (response severity < 0.80) are typically those with a $KLa1$ value near zero (normalised value in the region 0.03 – 0.19, equivalent to $0.7 - 4.6 \text{ d}^{-1}$) and a normalised $KLa2$ value less than 0.54 (equivalent to 13.0 d^{-1}). Solutions with the highest $KLa1$ and $KLa2$ values exhibit poor robustness: Those with a high $KLa1$ all result in effluent quality failure within the given disturbance magnitude, and a high $KLa2$ value also corresponds with either failure or a very high response severity. This is as expected, since aeration of the first activated sludge reactors is unconventional and would affect denitrification. Low levels of aeration may occur naturally as a side effect of mixing (Flores-Alsina et al. 2011), but these results suggest that low aeration levels in the first stages of the activated sludge unit should not be artificially implemented as a means of reducing GHG emissions, despite modelling suggesting that, under design conditions, this could enable significant emission reductions whilst maintaining a compliant (albeit poor) effluent quality. As such,

it is recommended that future control strategy optimisation should not consider aeration intensities in the ‘anoxic’ tanks as decision variables.

To enable a more detailed analysis of factors contributing to a robust solution for the reduction of GHG emissions and the impact of control strategy optimisation, four solutions are compared with the base case in Figure 7.15. Solutions selected are those with the lowest OCI meeting the criteria detailed in Table 7.6, with solution 4 being the most robust. Outputs are normalised as in Figure 7.14.

Table 7.6: Characteristics of solutions compared in Figure 7.15

	GHG emission reduction with respect to base case	Robustness analysis failures	Reduction in worst case effluent quality response severity with respect to solution 1
Solution 1	10%	Any	N/A
Solution 2	10%	None	Any
Solution 3	10%	None	20%
Solution 4	10%	None	30%

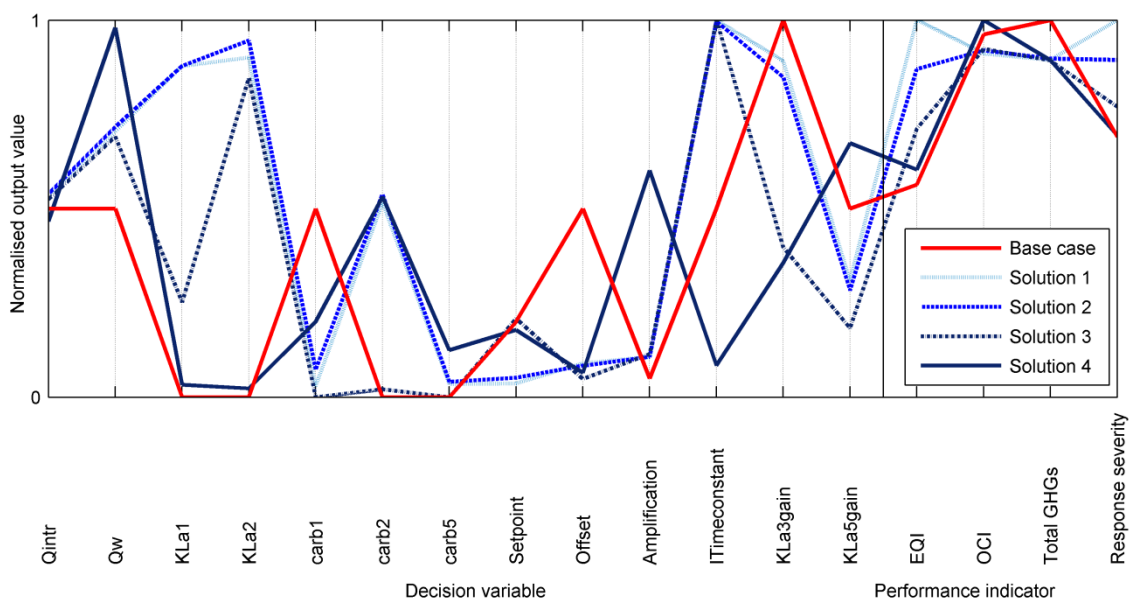


Figure 7.15: Comparison of decision variable values, key performance indicators and effluent quality robustness of base case and selected solutions providing a reduction in GHG emissions of at least 10%

Solutions 1, 2 and 3 achieve a 10% reduction in base case GHG emissions and operating costs simultaneously but the most robust solution (solution 4) requires an increase in operational costs. This does, however, provide the best effluent quality of the optimised solutions in addition to reducing the response severity.

Solutions analysed achieve a 10% emissions reduction with a wide range of $KLa1$ and $Kla2$ values, and these correspond with the trend noted for Figure 7.14: the most robust solutions have very low aeration intensities and best resemble standard operating practice for anoxic activated sludge reactors.

For all four solutions presented, Q_w is increased with respect to the base case. There is no clear connection between Q_w and robustness, however.

The most robust solutions have a DO setpoint near that of the base case ($2 \text{ g O}_2/\text{m}^3$), whilst cheaper and less robust solutions have significantly lower setpoints ($0.36 \text{ g O}_2/\text{m}^3$ and $0.52 \text{ g O}_2/\text{m}^3$ for solutions 1 and 2 respectively). This appears reasonable as a value of $2 \text{ g O}_2/\text{m}^3$ is commonly employed (e.g. Metcalf and Eddy 1994), although lower values may be used (e.g. Wanner 1994). Of the optimised solutions providing an emission reduction of at least 10%, 93% of those which utilise a DO setpoint less than $0.5 \text{ g O}_2/\text{m}^3$ exhibit unsatisfactory robustness, as shown in Figure 7.16. In order to develop a robust control solution, therefore, a minimum DO setpoint of $0.5 \text{ g O}_2/\text{m}^3$ is recommended. Continued increase in DO setpoint does not necessarily improve robustness and solutions with a setpoint in the range $0.5 - 1.0 \text{ g O}_2/\text{m}^3$ have a similar effluent quality response severity to those with a setpoint greater than $2 \text{ g O}_2/\text{m}^3$.

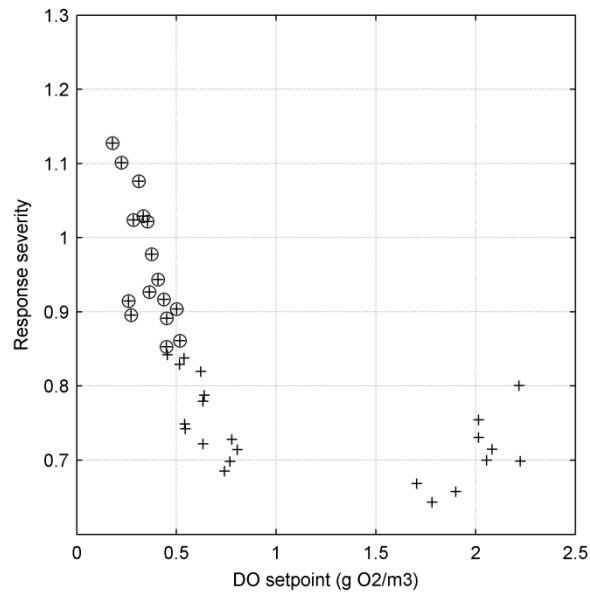


Figure 7.16: Relationship between DO setpoint and worst case effluent quality response severity for solutions providing a reduction in GHG emissions of at least 10%, with solutions which reach failure point circled

Generation Comparison

To assess the impacts of control strategy optimisation on robustness and determine whether less heavily optimised solutions are preferable, the most severe effluent quality response and associated failures for non-dominated solutions from generations 10, 15, 20 and 25 (final generation) are shown in Figure 7.17.

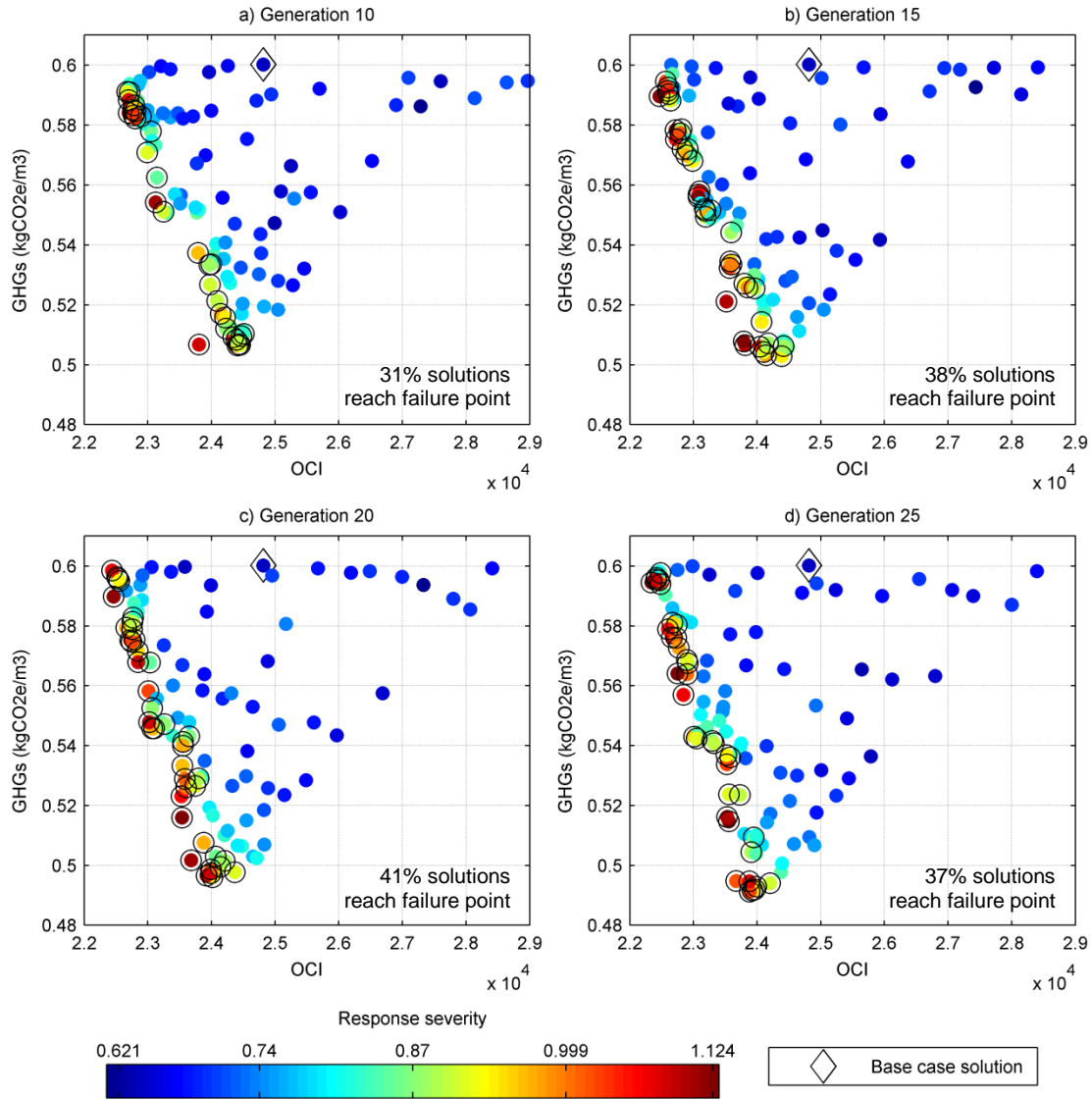


Figure 7.17: Worst case effluent quality response severity for non-dominated solutions which better the base case GHG emissions under default conditions from generations 10, 15, 20 and 25, with solutions which reach failure point circled

Despite the proportion of solutions which reach failure point increasing through the optimisation process, significant improvements in the position of the Pareto front are also observed. In each generation the least robust solutions are those on or near the GHG/OCI Pareto front, but solutions are found behind the Pareto front in generation 25 which provide a similar level of GHG and OCI reduction to those on the generation 10 Pareto front and are more robust.

Optimised solutions in all generations typically have a greater effluent quality response severity than the base case, but solutions which do not reach failure

point within the given disturbance magnitude are deemed to still provide an acceptable level of robustness. On the basis of these results, control strategy optimisation is not thought to be severely detrimental to robustness, since it enables identification of solutions which provide similar performance under design conditions to less highly optimised solutions, but with a higher degree of robustness. Whatever the degree of optimisation, however, it is important to consider the robustness of control strategies, as those which appear to perform best under design conditions may not be sufficiently robust.

7.5 Resilience of Optimised Control Strategies

7.5.1 Resilience Assessment Methodology

Analysis of resilience is carried out for all 100 final generation solutions for which reliability and robustness were assessed. These all better the base case GHG emissions whilst maintaining a compliant effluent when evaluated under default conditions.

It is necessary to define resilience of *what* to *what*. As for reliability and robustness, this study investigates the resilience of effluent quality compliance and GHG emissions. In terms of resilience *to what*, it is suggested that control strategies need to be assessed with respect to acute threats rather than gradual change, a) because resilience implies that recovery occurs, and recovery is unlikely to occur under the same control strategy if the disturbance is not removed; and b) because under long term changes it is unlikely that the same, sub-optimal control strategy would remain in use – modifications would be made to the system to improve performance. Therefore, it is not possible to assess resilience to the same threats as were considered for robustness (perturbations in influent flow rate, influent total nitrogen concentration, influent COD concentration and temperature) unless a specific event which results in only temporary occurrence of such perturbations is defined. Definition and modelling of such events would be complex due to the high degree of associated uncertainty – for example, temporarily increased flow rate may occur as a result of a storm event, but in order to model resilience to storm events it would be necessary to assign probability functions their magnitude, duration, time of occurrence and frequency, and relate all of these to the WWTP influent flow rate (and potentially other influent parameters which may be affected). An

alternative, but useful, acute threat to which resilience can be assessed is sensor failure. This is an important consideration given that, for the purposes of optimisation, WWTP performance was assessed assuming ideal sensors (i.e. no noise or delay, and no failures) but in reality failures are likely to occur at some stage.

This section of the work, therefore, aims to investigate the resilience of BOD₅, COD, total nitrogen, TSS and GHG emissions from optimised control strategies to sensor failure.

Modelling Sensor Failure

Modelling of sensor faults is based on the example given by Rosen et al. (2008), in which four sensor states are considered: fully functional, complete failure, wrong gain and in calibration. During normal operation, sensor measurements are only affected by normal noise. When fully operational, the sensor may remain operational, move to a state of complete failure or enter calibration. During complete failure, the sensor either has no output signal or the output takes the minimum value. When in calibration, the sensor provides an incorrect measurement, which can be modelled as for a complete failure. Following calibration, the model may either return to a fully functional state or have the wrong gain; wrong gain can only occur as a result of incorrect calibration and can only be corrected by further calibration.

Transition probabilities between each state are used to produce sensor state time series. Probabilities calculated by identification of fault types in 286 days of online ammonia measurement from a Swedish treatment plant (Rosen et al. 2008) are presented using a Markov chain representation, shown in Figure 7.18. These transitional probabilities are used as the basis for sensor fault modelling in this study. Whilst it is recognised that fault probabilities may differ to some extent between sensor types and between individual sensors, it is not possible to obtain site specific data given that the plant under study is hypothetical. These figures are considered sufficient to provide an indication of realistic sensor behaviour.

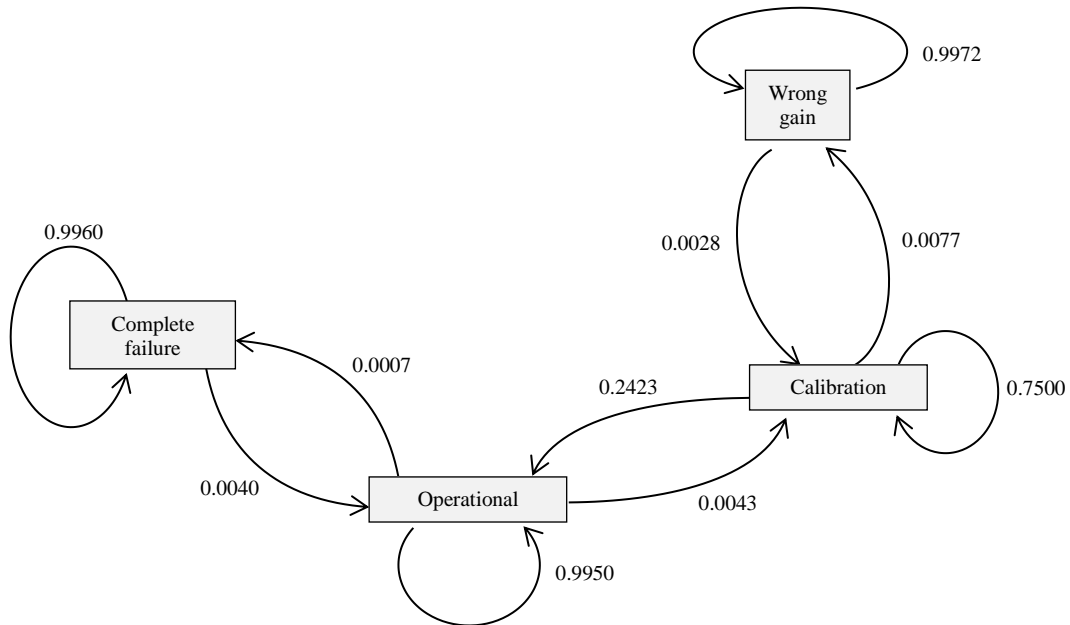


Figure 7.18: Markov chain representation of the sensor fault model used by Rosen et al. (2008)

Modelling wrong gain as a failure state requires the incorrect gain to be defined; in the example given (Rosen et al. 2008), however, the values relate to an ammonium sensor and may not be appropriate for a DO sensor. Therefore, in modelling the effects of sensor failure on effluent quality and GHG emissions for assessment of control strategy resilience, only two sensor states are considered: operational (O) and failure (F). The probability of transitioning to each state at each time step, given a known current state, is represented in Figure 7.19. Transition probabilities are taken from Figure 7.18, with the exception of $P(O|O)$; this now incorporates the 0.0043 probability that the sensor will transition from operational to calibration status, since calibration is no longer considered.

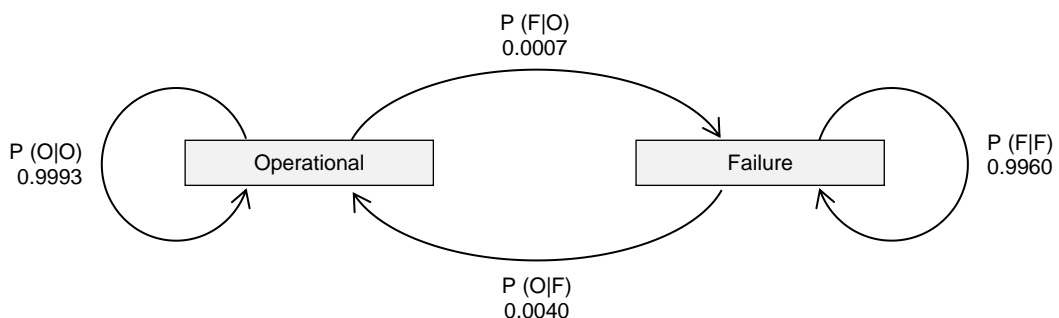


Figure 7.19: Markov chain representation of the sensor fault model used in this study

Using these transition probabilities, 500 14-day sensor state time series with 15 minute intervals are generated. In each case, the initial state is selected based on the overall percentage of time in failure mode reported by Rosen et al. (2008):

$$P(F) = 0.14$$

$$P(O) = 0.86$$

An overview of the characteristics of 500 sensor state time series generated for evaluation is given in Table 7.7. The sensor remains fully operational for the entire 14 day period in 36.2% of the samples; in the remaining, up to four individual periods of sensor failure occur. Examples of the sensor state time series are given in Figure 7.20, where 1 denotes fully operational and 0 denotes failure state.

Table 7.7: Overview of sensor failure characteristics

	Individual failure events	Total failures in each 14 day sample
Mean duration (days)	2.29	2.15
Minimum duration (days)	0.01	0.00
Maximum duration (days)	12.41	12.67
Minimum number of failures	-	0
Maximum number of failures	-	4

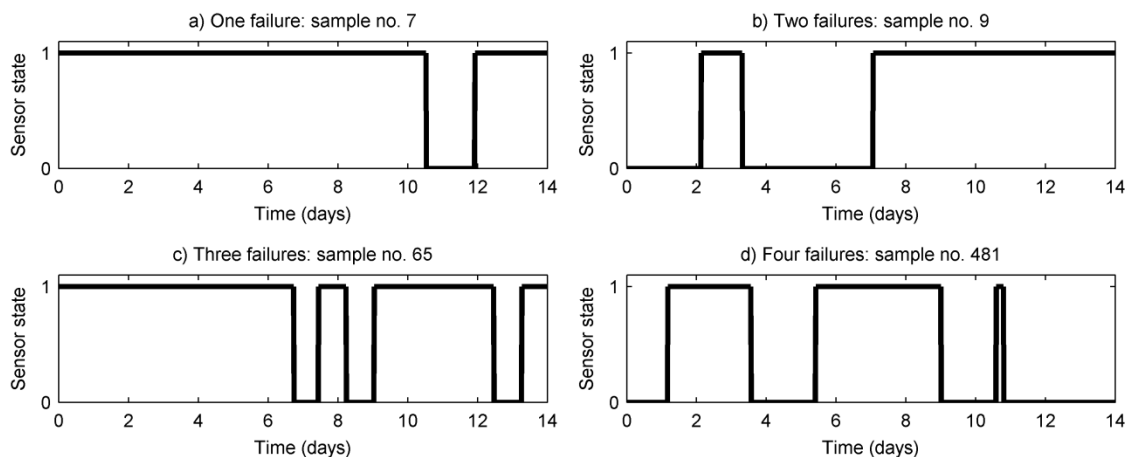


Figure 7.20: Example sensor state time series

Control Strategy Performance Modelling under Sensor Failure

Each solution is evaluated using each of the 500 sensor state time series, resulting in 5,000 scenarios for simulation. Simulations are carried out as for the multi-objective optimisation, with the exception of sensor modifications. The ideal sensor is replaced with a non-ideal sensor, which includes modelling of noise as in BSM2 (Alex et al. 2008), and modelling of sensor failures corresponding to the relevant sensor state time series. Sensor faults are implemented in the sensor model (shown in Figure 7.21) using a fault vector by which the sensor output is multiplied: '1' denotes fully operational at a given time step and '0' denotes failure, thereby producing a sensor output of zero during failure.

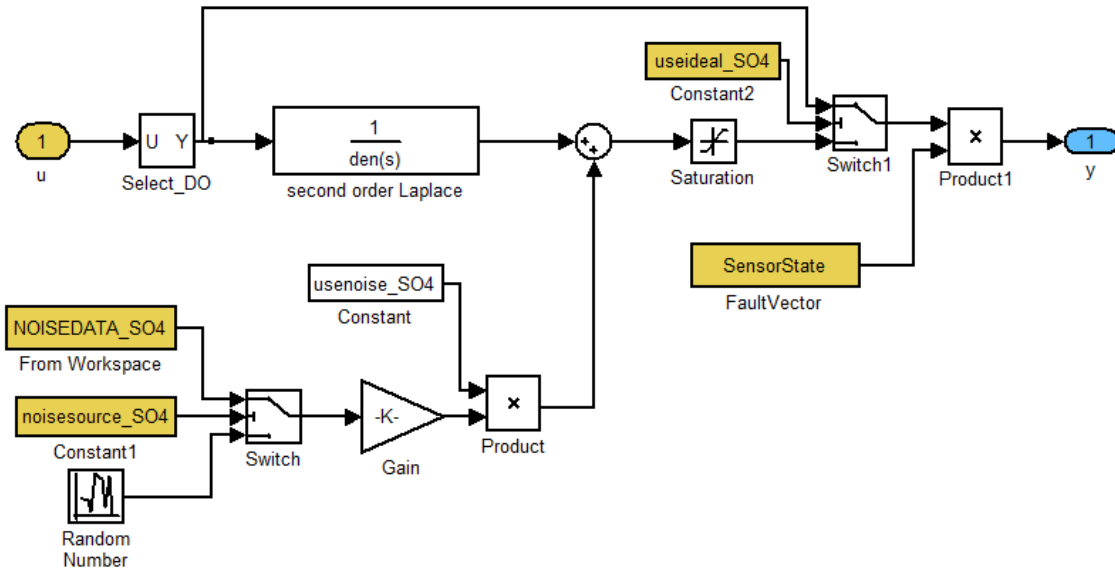


Figure 7.21: Implementation of fault modelling in DO sensor

For each simulation, dynamic plant performance during the final seven days of the winter and summer evaluation periods is recorded and stored for calculation of resilience indicators.

Calculation of Resilience Indicators

Resilience indicators are calculated as detailed in Section 7.2.2 for each solution when subject to each of the 500 sensor state time series. Each solution, therefore, has $500 \times 3 \times 5 = 7500$ associated indicator values: R_V , R_{T1} and R_{T2} for each of the key model outputs (BOD₅, COD, total nitrogen, TSS and GHG emissions) for each sensor state time series. Overall resilience indicators

for each model output of each solution are calculated as the median of values calculated under each of the 500 sensor state time series.

Failure limits listed in Table 7.5 are used for the effluent quality indicators. It is noted that these limits, as defined in the UWWTD, are either 95 percentile (for BOD₅, COD and TSS) or mean (for total nitrogen values) and exceedance for a short duration is technically acceptable. In the context of dynamic performance, however, it is not possible to pinpoint the precise moment at which limits for percentile or mean performance is breached – they are, therefore, assumed to be absolute limits for the purpose of resilience assessment. A dynamic failure limit is set for GHG emissions, equal to emissions under the base case control strategy at each time step.

7.5.2 Resilience Assessment Results and Discussion

No effluent BOD₅, COD or TSS failures are observed for any control solution under any of the sensor state time series analysed. Correspondingly, for these performance indicators, all solutions have an R_V value of one, and R_{T1} and R_{T2} values of infinity. Therefore, all solutions can be said to have an effluent BOD₅, COD and TSS which is resilient to sensor failure. Failures are observed in both effluent total nitrogen and GHG emissions, although for some solutions the median R_{T1} and R_{T2} resilience indicators are infinity since failures do not occur in every sample. Results not presented in this chapter, showing R_V , R_{T1} and R_{T2} values for each solution based on effluent total nitrogen and GHG emissions, are provided in Appendix F.

Effluent Total Nitrogen Resilience

A comparison of nitrogen resilience indicators is given in Figure 7.22. To enable visualisation of the resilience of all solutions, R_{T1} infinity values are displayed as 20,000 and R_{T2} infinity values are displayed as 20. There is a very strong correlation ($r = 1.00$) between R_{T1} and R_{T2} , suggesting that either can be used to provide a good measure of resilience for system response and recovery. There is also a strong positive correlation between R_V and R_{T1} and R_{T2} and solutions with a very high resilience for system response and recovery all have an R_V value greater than 0.98. However, solutions exist with an R_V value greater than 0.98 but an R_{T2} value less than 1.75 (placing them in the bottom 50 percentile for this indicator). Solutions are, therefore, analysed on the basis of

resilience for system response and recovery, since this provides a more conservative measure of their resilience.

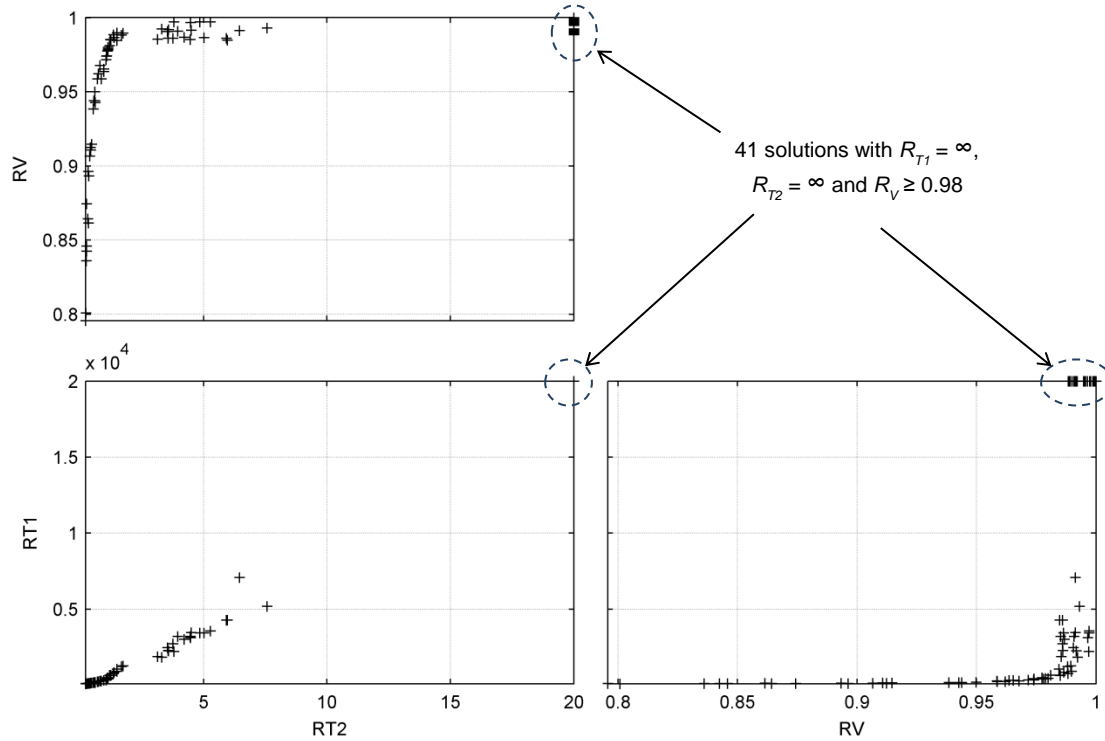


Figure 7.22: Comparison of resilience indicators based on effluent total nitrogen

Effluent total nitrogen resilience indicators (R_{T2}) for each solution are presented in Figure 7.23. A high proportion of solutions have an effluent nitrogen concentration which is highly resilient to sensor failure, achieving R_{T1} and R_{T2} values of infinity; these are typically solutions with lowest EQI under design conditions. Optimised solutions on the GHG/OCI Pareto front (which have a high EQI) perform poorly when subjected to sensor failures. It is inadvisable, therefore, to implement solutions which appear to offer the greatest reduction in GHG emissions and the lowest costs, although significant improvements may still be made at little additional cost whilst maintaining a high level of resilience.

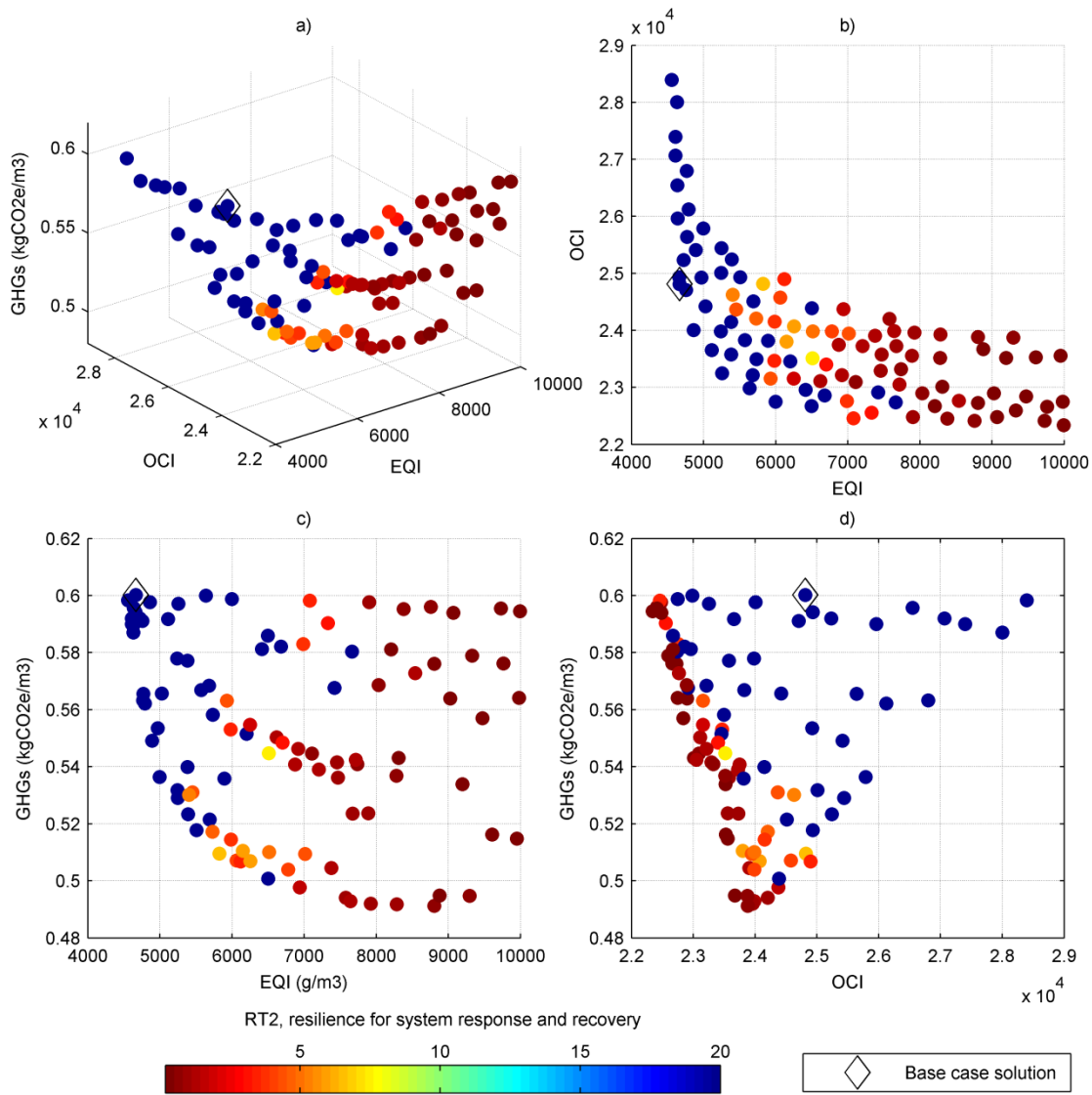


Figure 7.23: Resilience for system response and recovery (R_{T2}) (effluent total nitrogen) for non-dominated solutions bettering base case GHG emissions under default conditions; solutions with $R_{T2} = \infty$ are shown as $R_{T2} = 20$

Analysis of the characteristics of each solution shows that there are no significant correlations between decision variable values and any effluent total nitrogen resilience indicators (greatest correlation coefficient, $r = -0.20$). Figure 7.24 shows decision variable values for two sets of solutions providing a 10% reduction in GHG emissions: 1) solutions with high total nitrogen resilience ($R_{T2} = \infty$); and 2) solutions with low total nitrogen resilience ($R_{T2} < 1$). Even here, however, there is no clear distinction between the high resilience and low resilience solutions. As such, no specific recommendations can be made regarding control strategy design features for effluent quality resilience to sensor failures. However, the relationship between EQI and resilience shows

that control strategies must be designed to produce an effluent quality under design conditions that is considerably better than the minimum required for compliance if they are to have satisfactory effluent quality resilience.

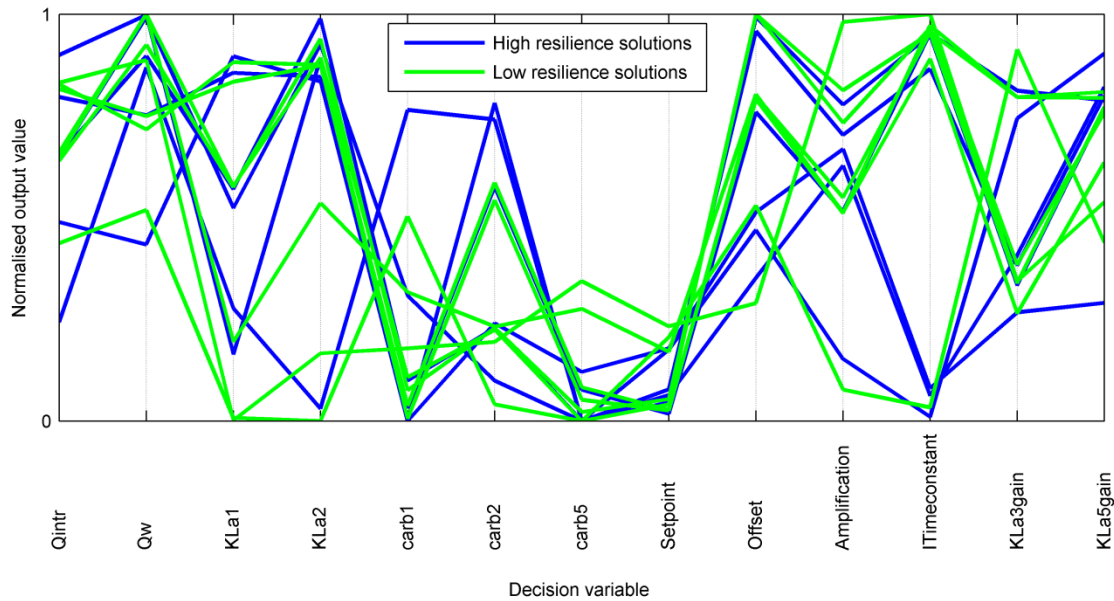


Figure 7.24: Comparison of decision variable values of providing a reduction in GHG emissions of at least 10% with high total nitrogen resilience and poor total nitrogen resilience

Greenhouse Gas Emission Resilience

The relationship between resilience indicators is less distinct for GHG emissions than for effluent total nitrogen, as shown in Figure 7.25, so at least two indicators (one for resilience against crossing a performance threshold and another for system response and recovery) are required to give a complete picture of the resilience of GHG emissions to sensor failure. These are shown in Figure 7.26 and Figure 7.27. R_{T2} is selected for resilience for system response and recovery, based on previous recommendation (Kundzewicz and Kindler 1995).

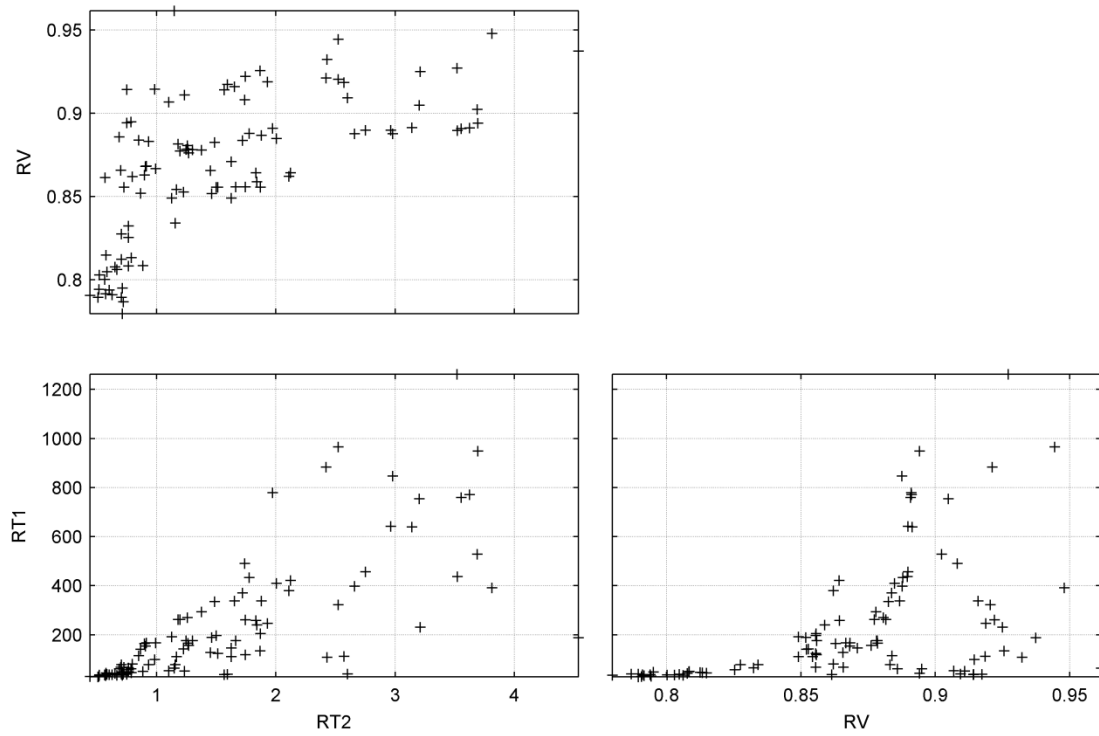


Figure 7.25: Comparison of resilience indicators based on GHG emissions

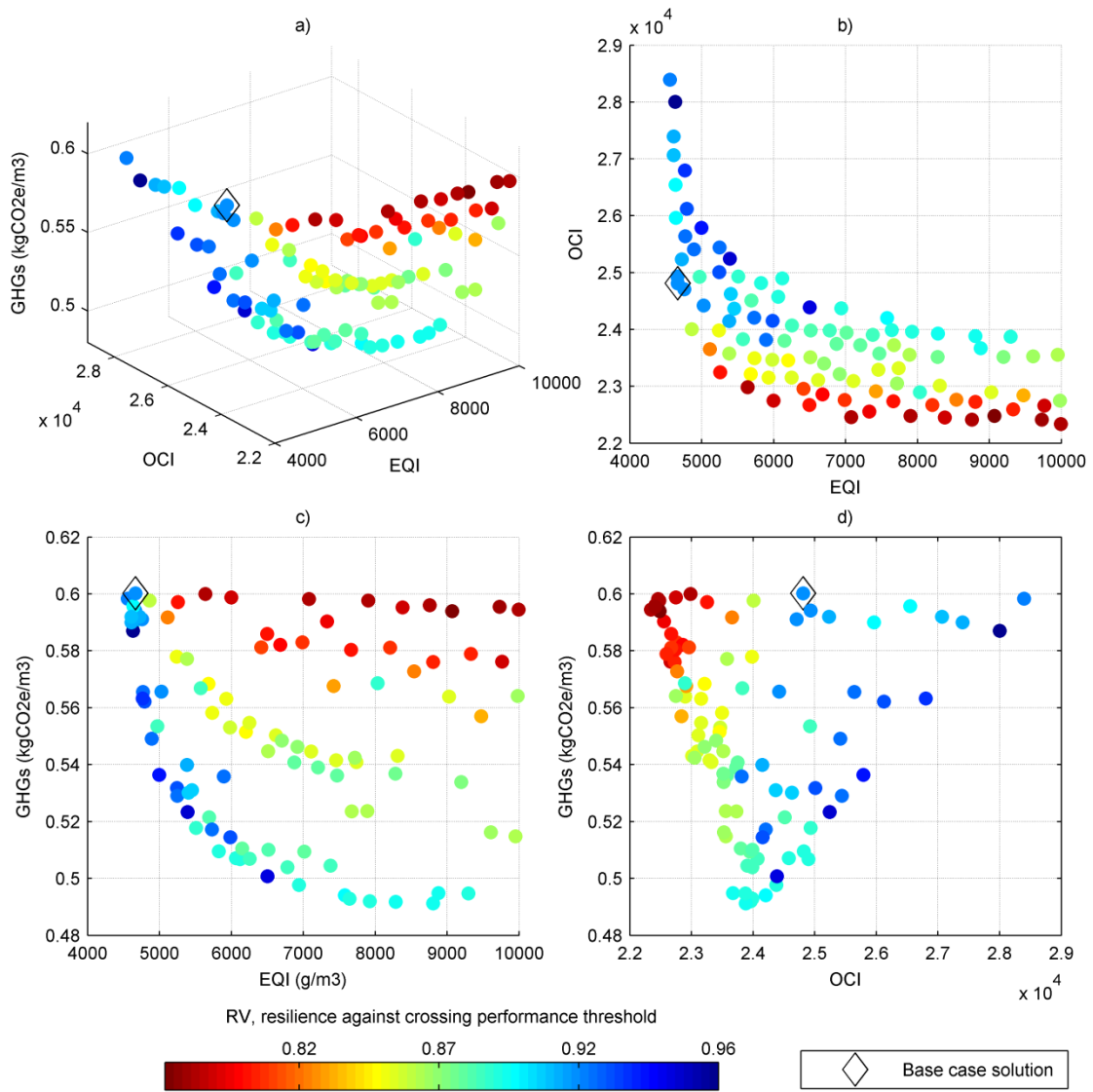


Figure 7.26: Resilience against crossing a performance threshold (GHG emissions) for non-dominated solutions bettering base case GHG emissions under default conditions

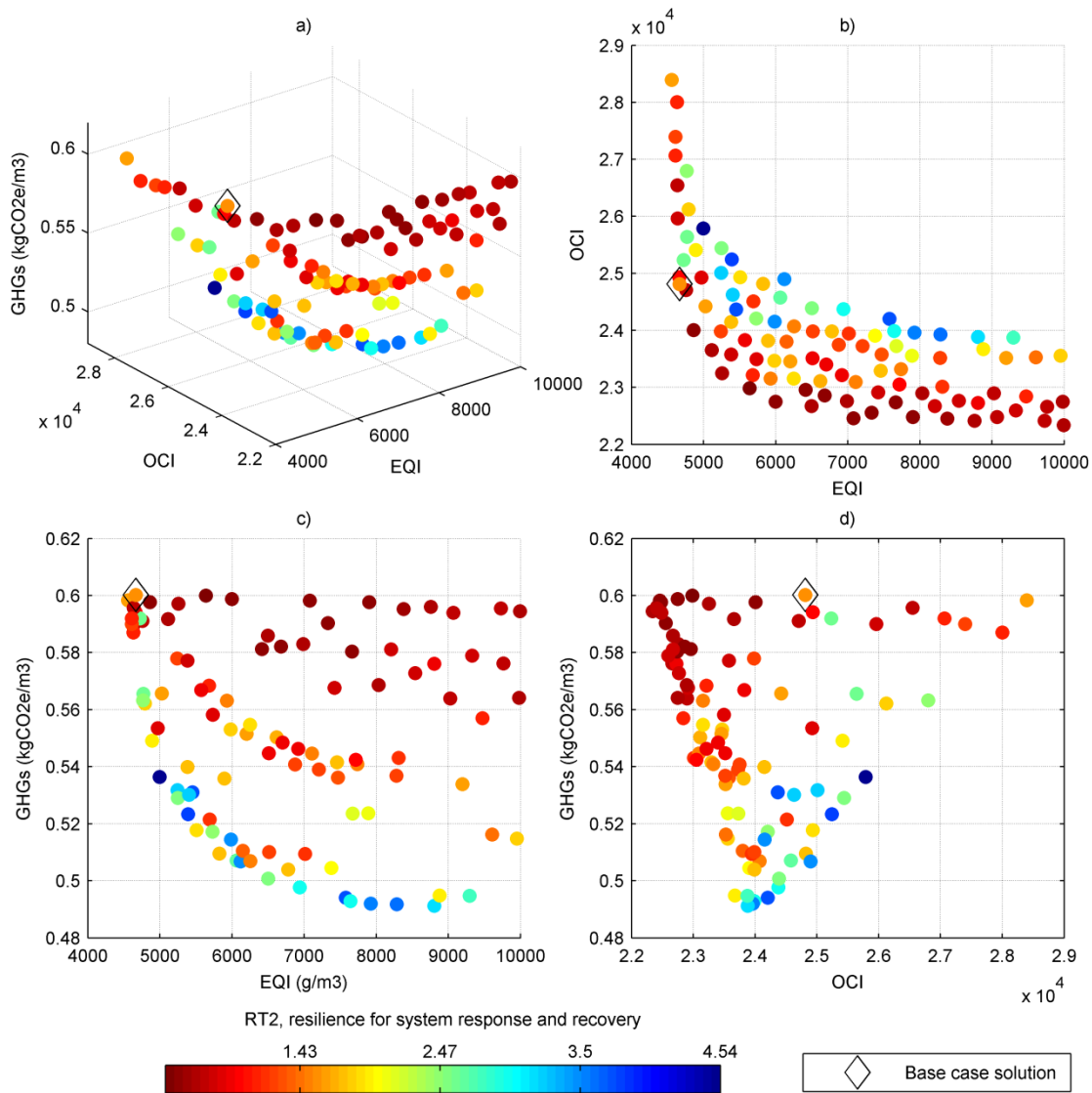


Figure 7.27: Resilience for system response and recovery (R_{T2}) (GHG emissions) for non-dominated solutions bettering base case GHG emissions under default conditions

Solutions with lowest operational costs exhibit the lowest resilience against crossing a performance threshold (Figure 7.26). These solutions also provide little reduction in GHG emissions and a higher EQI than the base case, and would be unlikely candidates for implementation due to their small potential benefit (in terms of emission reduction) and the demonstrated impact of a high EQI on effluent quality reliability, robustness and resilience.

Figure 7.29 shows a similar trend, with solutions with a low OCI providing poor resilience for system response and recovery. However, it is also clear that solutions which provide little reduction in base case GHG emissions offer little resilience to sensor failure, whilst those with the greatest emission reduction are

significantly more resilient. This is as expected since the failure limit is equal to base case emissions under design conditions, so solutions with the greatest reduction in emissions are typically less likely to cross this limit following sensor failure.

Again, there are no strong correlations between decision variable values and any resilience indicators (greatest correlation coefficient, $r = 0.34$), so no conclusions regarding control characteristics which may contribute to a solution with high GHG emission resilience can be drawn.

7.6 Comparison of Control Strategy Reliability, Robustness and Resilience

This section explores the relationships between reliability and robustness and between reliability and resilience, and aims to identify common features of the most reliable, robust and resilient design solutions. The connection between robustness and resilience is not investigated since these are assessed with respect to different threats. The validity of sensor failure (as considered in resilience analysis) as a threat in robustness analysis would be questionable, given that a range of disturbance magnitudes should be modelled and a specific disturbance magnitude resulting in failure must be identifiable. It is uncertain whether a relationship between the robustness and resilience of solutions, as calculated in this study, would be expected – or what its relevance would be if observed.

Comparisons between reliability and robustness indicators, based on effluent quality and GHG emissions, are given in Figure 7.28 and Figure 7.29 respectively. Solutions which do not reach failure point in robustness analysis (classified as ‘acceptable robustness’) are identified and, for the effluent quality, solutions providing an acceptable (compliant) level of reliability are also shown.

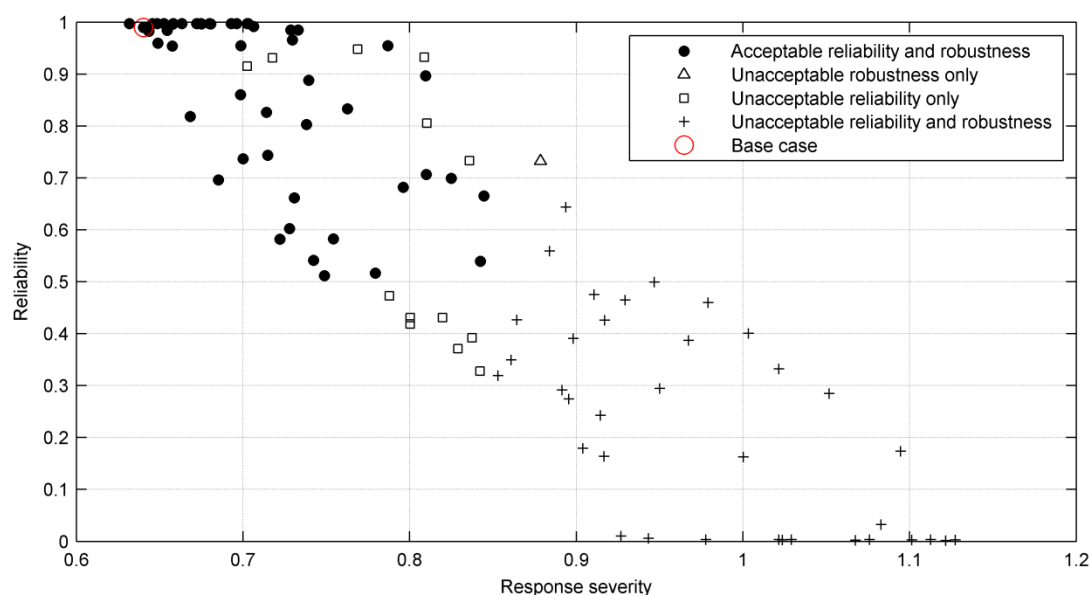


Figure 7.28: Comparison between worst case effluent quality response severity and reliability

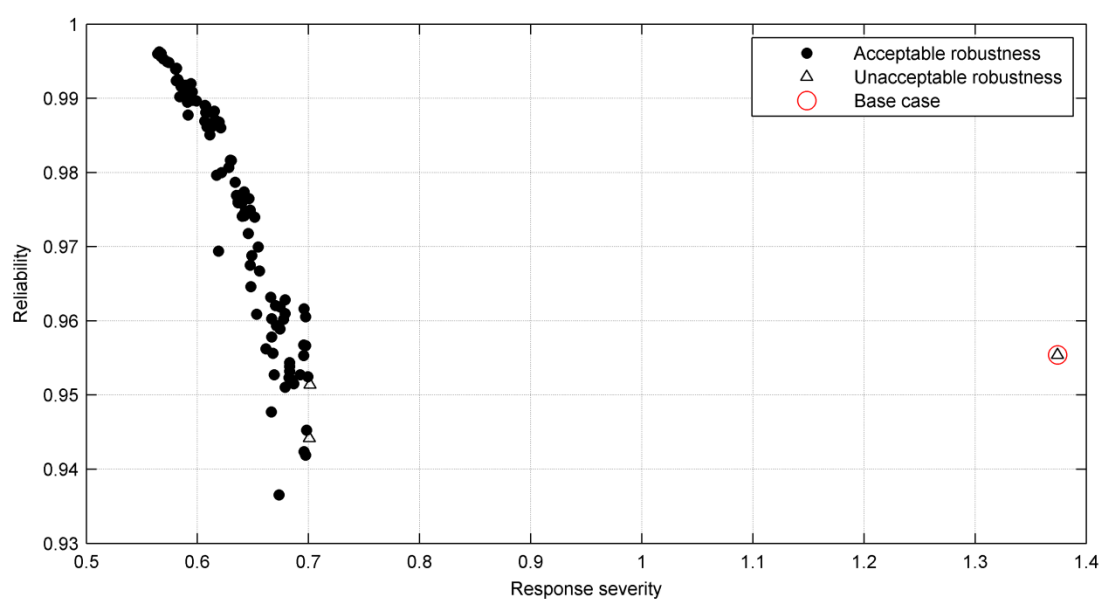


Figure 7.29: Comparison between worst case GHG emission response severity and reliability

For both effluent quality and GHG emissions, a very strong correlation between reliability and robustness is observed, suggesting that designing to achieve a high degree of reliability will provide a solution with a high degree of effluent quality and GHG emission robustness to perturbations in influent flow rate, COD, total nitrogen and temperature. Only 1% of solutions provide an acceptable effluent quality reliability yet still reach failure point in robustness

analysis, and the least robust solutions are those with unacceptable reliability. However, Figure 7.28 also shows that, whilst a high degree of effluent quality reliability can be maintained during control strategy optimisation to reduce GHG emissions, a decrease in robustness (i.e. increase in response severity) with respect to the base case is a likely trade-off.

Comparisons between reliability and the R_{T2} resilience indicators are given in Figure 7.30 and Figure 7.31. R_{T2} values are limited to a maximum of 20 to aid visualisation, and solutions with an original R_{T2} value of infinity are classified as 'highly resilient' and identified in the figures. Solutions providing an acceptable level of effluent quality reliability are also identified in Figure 7.30.

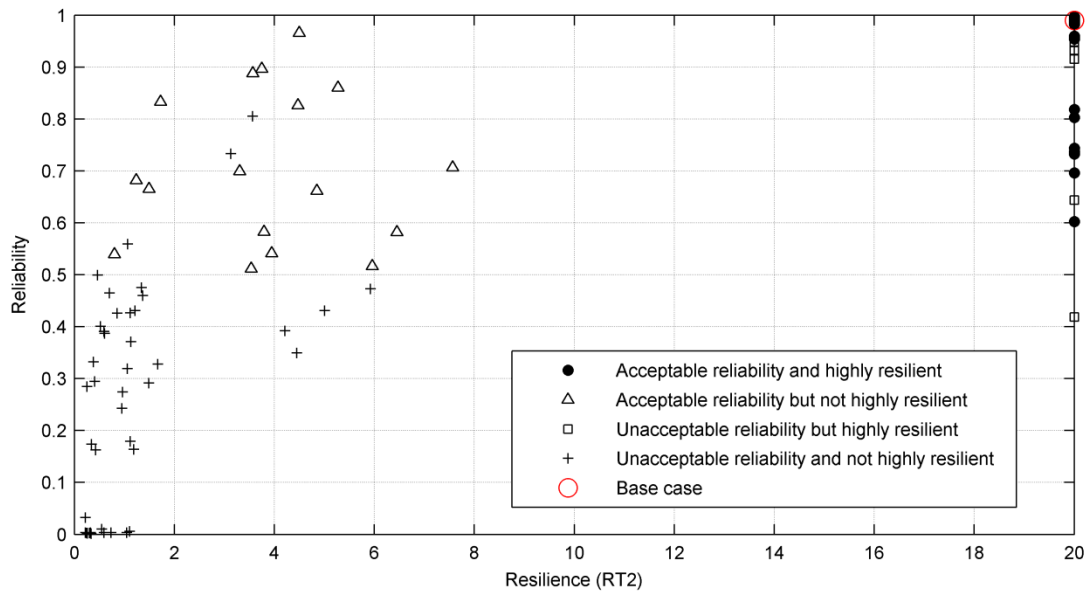


Figure 7.30: Comparison between worst case effluent quality resilience (indicator R_{T2}) and reliability

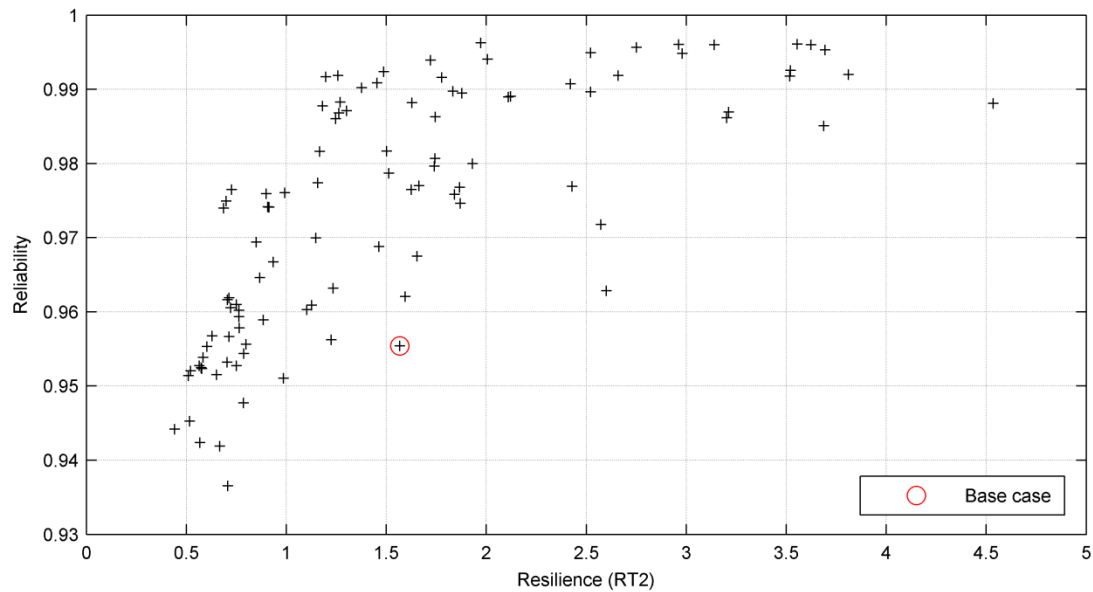


Figure 7.31: Comparison between GHG emission resilience (indicator R_{T2}) and reliability

The correlation between effluent quality reliability and resilience to sensor failure (Figure 7.30) is weaker than for reliability and robustness, and there are many solutions which provide an acceptable level of reliability yet are not highly resilient. Solutions with unacceptable effluent quality reliability typically have a very low resilience to sensor failure, but there are also solutions with low resilience and acceptable reliability and, conversely, with high resilience and unacceptable reliability. It is important to note, however, that the criteria for a highly resilient solution are specified arbitrarily, and it may be that less resilient solutions are deemed acceptable.

There is a positive correlation between GHG emission reliability and resilience to sensor failures. However, optimised solutions with a similar level of reliability to the base case typically perform worse with respect to resilience. Such solutions are unlikely to be selected since the aim of optimisation is to reduce GHG emissions, but of those which improve upon the base case reliability, 50% also worsen resilience to sensor failures. It is suggested, therefore, that assessment of GHG emission resilience is used to guide control strategy selection in addition to GHG emission reduction under design conditions.

Figure 7.32 shows the performance of optimised solutions under design conditions with respect to EQI, OCI and GHG emissions, with solutions which provide an acceptable level of effluent quality reliability, no effluent quality

failures under influent perturbations in robustness analysis and a high level of resilience to sensor failure identified. Whilst the lowest emission solutions are unacceptable, an emission reduction of 13.7% can still be achieved whilst retaining satisfactory behaviour under design conditions and in response to threats.

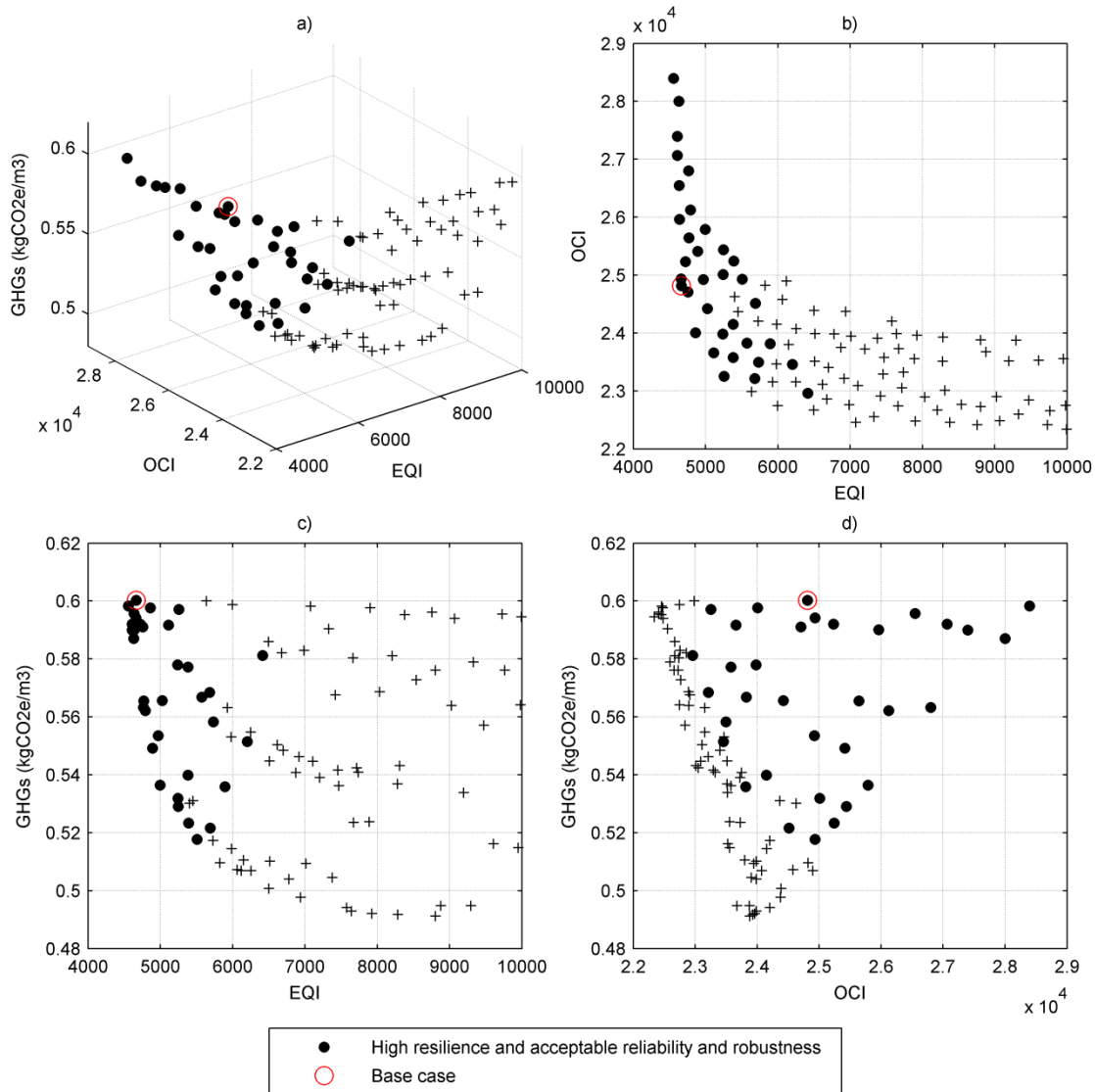


Figure 7.32: Comparison of performance under design conditions of solutions providing acceptable and unacceptable effluent quality reliability, robustness to influent perturbations and resilience to sensor failures

Solutions with the lowest EQI perform best, with all solutions with an EQI less than 5403 providing an acceptable level of effluent quality reliability, robustness and resilience. 82% of these solutions also have a mean effluent total nitrogen concentration of less than 10 g/m³. This is significantly below the UWWTD requirement, suggesting that in order to be reliable, robust and resilient in terms

of effluent quality, a design effluent total nitrogen below the regulatory standard is beneficial.

Analysis of decision variable values shows that all solutions with a *carb5* value greater than 0.14 g/m^3 and/or a *KLa1* value greater than 12.5 d^{-1} provide unacceptable effluent quality reliability, robustness and/or resilience. Conventionally, carbon source addition is only applied to anoxic tanks, to provide the required COD/N ratio for denitrification, and these tanks are not aerated. It is suggested that aeration intensities in 'anoxic' tanks and carbon source addition rates in aerated tanks are not included in future optimisation, despite their observed effects on EQI, OCI and/or GHG emissions in sensitivity analysis.

7.7 Conclusions

This research has assessed the reliability, robustness and resilience of optimised control strategy effluent quality and GHG emissions with respect to specific threats, and distinguished between features which contribute to desirable and less desirable solutions. Whilst it must be noted that this research is based on the study of a single WWTP only and further, case-specific investigation should be carried before applying this knowledge to other sites, the following key conclusions are drawn:

- Multi-objective control strategy optimisation to minimise effluent pollutants, operational costs and GHG emissions enables development of solutions which significantly reduce GHG emissions and maintain a compliant effluent with a high degree of reliability, robustness (with respect to influent disturbances) and resilience (with respect to sensor failure). However, not all solutions are reliable, robust and resilient, and further analysis is required beyond the optimisation process to ensure that implemented solutions produce acceptable performance when subject to threats.
- Solutions with a low EQI have the highest effluent quality reliability, robustness and resilience. Those which fail to reach an acceptable level of effluent quality reliability, robustness or resilience predominantly do so due to the occurrence of elevated nitrogen concentrations. Therefore, solutions should be designed to provide an effluent quality (in particular,

effluent nitrogen) under design conditions which is significantly better than that required for compliance. If optimisation tools are to be used for control strategy development then effluent quality constraints must be stricter than the legislative limits.

- Solutions which are predicted to achieve the most significant improvements in GHGs and OCI under design conditions typically have a poor effluent quality and may perform poorly in reality when subject to threats.
- A DO setpoint below 0.64 g/m^3 typically corresponds with unacceptable effluent quality reliability. A setpoint of above 0.5 g/m^3 is required to ensure acceptable effluent quality robustness, but significant further increase in setpoint offers little benefit in terms of robustness.
- Aeration intensities in 'anoxic' reactors and carbon source addition in aerated reactors should not be considered as decision variables in optimisation of this plant, unless it is converted to a post denitrification plant. Low/no aeration in the first activated sludge reactors is preferable in terms of effluent total nitrogen reliability and high aeration intensities also result in poor effluent quality robustness. Solutions with high carbon source addition in the aerobic reactors fail to provide a reliable, robust and resilient design.

8 GUIDELINES FOR THE DEVELOPMENT OF CONTROL STRATEGIES TO REDUCE GREENHOUSE GAS EMISSIONS

8.1 Introduction

It has been shown that a reduction in GHG emissions resulting from WWTP operation can be achieved with improved control and this chapter draws upon the findings in Chapters 4-7 to produce guidance for WWTP operation and development of control strategies for emission reduction at an acceptable cost whilst maintaining legislative compliance, taking into account the effects on reliability, robustness and resilience. The intention is not to prescribe a specific control strategy or changes that can be implemented to guarantee a reduction in emissions, rather to suggest approaches to control strategy development that may be used and to identify key control features for consideration and testing in a case-specific context.

The guidelines are deliberately general and, given that they are based on the study of only a single, hypothetical plant, it is unclear how effective they will be when applied to different scenarios. Evaluation of newly developed control strategies on a site specific basis is vital to gain an understanding of the effects of modifications under different situations. The effects of omissions in the sources of GHG emissions modelled and other modelling uncertainties must also be considered in the implementation of these guidelines, and these are discussed in Section 8.6.

8.2 Emission Sources

In the development of strategies to reduce GHG emissions, this research has demonstrated the importance of considering all sources of emissions, both direct and indirect, not just those which must be reported under the CRC. It is possible that some options which can be implemented to reduce total GHG emissions at a low cost and whilst maintaining a good quality effluent actually result in an increase in net energy use, since reduced energy recovery from biogas combustion can be offset by a reduction in emissions associated with sludge disposal; however, the CRC disincentivises such solutions. There are also instances in which a reduction in emissions reported under the CRC results in an increase in net emissions, further highlighting the importance of accounting for emissions from all sources.

Control handle sensitivity analysis has shown that N₂O emissions from the activated sludge reactors are the greatest contributor to variance in total GHG emissions, suggesting that this is the source with greatest potential for improvement and that any significant reduction in GHG emissions achievable with modified control alone will be primarily due to a reduction in N₂O emissions. Therefore, it is important that N₂O emissions are modelled accurately and the model should be calibrated with N₂O emission data if possible. Following any changes in control, it is important that N₂O emissions are monitored to ensure that they have not been inadvertently increased.

8.3 Key Control Handles and Decision Variables

This section aims to identify control handles and decision variables which are important to consider in future control strategy modifications, as well as those which have been found to result in little benefit and are low priority for adjustment. Multi-objective optimisation has shown that a significant reduction in GHG emissions can be achieved with many different combinations of decision variable values. Where appropriate, general recommendations regarding the values (high/low, increase/decrease etc.) are made based on analysis of improved solutions developed in this study but, unless effluent quality and/or operational costs are to be worsened, it will be necessary to consider the effects of implementing multiple changes simultaneously.

It is important to note that these recommendations are based on the study of a single activated sludge plant; a different system may contain additional potential decision variables, and those identified as important here may be less influential than expected. However, they provide a basis for further development.

8.3.1 High Priority for Investigation

Wastage Flow Rate

Selection of a suitable wastage flow rate is of key importance. GHG emissions, operational costs and effluent quality are all highly sensitive to adjustments in this control handle value, and this is evidenced by the variability of performance indicators recorded for solutions with a range of sampled wastage flow rates throughout the year.

Implementation of different wastage flow rates throughout the year in order to maintain sufficient biomass in the system is standard practice. However, selection of appropriate values can aid the reduction of GHG emissions. There are contrasting approaches to this, each of which affects different emission sources. Firstly, emissions reduction can be achieved with high wastage flow rates (and a low SRT). This provides a moderate decrease in both N_2O and non- N_2O emissions from activated sludge. Secondly, emission reduction can be achieved with low wastage flow rates (and a high SRT), which results in an increase in energy costs (due to increased aeration) and non- N_2O activated sludge emissions but a significant reduction in N_2O emissions. Low SRT solutions require a trade-off in effluent quality and may cause an increase in N_2O emissions from sources not modelled in this research. Excessively high wastage flow rates may also prevent a stable population of bacteria forming and result in washout (Grady et al. 1999).

Given the greater reduction in N_2O emissions achieved with high SRT solutions, and the high contribution of uncertainty in direct N_2O emissions to uncertainty in total modelled GHG emissions, it is suggested that a low wastage flow rate solution is preferable and opportunities for reduction of wastage flow rate should be explored when modifying WWTP control. This is likely to increase energy use and non- N_2O emissions from activated sludge (Flores-Alsina et al. 2011, Sweetapple et al. 2014c), and so will be undesirable under the CRC, but should reduce net GHG emissions.

When implementing these changes, it is important that standard design considerations are not overlooked. Wastage flow rates should be selected so as to provide SRT values within the normal operating range; these can typically be as high as 15 days for a complete mix process, 30 days for an oxidation ditch or 40 days for an extended aeration process (Metcalf and Eddy 1994). Insufficient wastage can result in problems such as low F/M bulking (Ma and Peng 2006), which were not modelled in this research, and the risk of such issues should be assessed before implementation of changes.

Aeration Intensities and Dissolved Oxygen Setpoint

In the WWTP studied, GHG emissions are found to be sensitive or highly sensitive to aeration intensities in all aerobic reactors, with effluent quality and

operational costs also affected significantly by aeration in the final reactor(s). In future control strategy development, selection of appropriate aeration intensities is of key importance and it is recommended that active control of these control handles (using one or more DO setpoints, as discussed in Section 8.4) is implemented. It is vital that the impacts of any modifications are assessed with respect to effluent quality and operational costs in addition to GHG emissions, however, as aeration has significant individual impacts on all three performance indicators, as well as contributing to interaction effects. It is also important that changes in aeration are assessed in conjunction with any other modifications implemented since aeration intensities are involved in significant interaction effects with, for example, wastage flow rate.

It is widely recognised that selection of an appropriate DO setpoint is highly important in terms of the effects on GHG emissions as well as on effluent quality and operational costs (e.g. Flores-Alsina et al. 2014). In this research, solutions found to perform best with respect to emissions and costs whilst retaining a compliant effluent quality have a low DO setpoint ($0.5 \text{ g O}_2/\text{m}^3$) in the final activated sludge reactor when controlling each reactor individually, whilst too high a setpoint is found to increase GHG emissions and operational costs. It is suggested, therefore, that the effects of DO setpoint reduction are investigated when attempting to reduce GHG emissions.

A reduction in DO setpoint has the potential to reduce N_2O emissions in particular, since denitrification enzymes can be inhibited by the presence of oxygen, preventing complete denitrification. This effect has been observed previously by Aboobakar et al. (2013). Reduced aeration also results in less N_2O being stripped to the atmosphere (Guo et al. 2012b). However, it is also important that sufficient DO is maintained for nitrification in order to minimise N_2O emissions from alternative sources; previously, increased N_2O emissions have actually been reported under a low DO setpoint (Guo et al. 2012b) and it has been suggested that a minimum DO concentration of $0.5 \text{ g O}_2/\text{m}^3$ should be maintained (Zheng et al. 1994).

Analysis of optimised solutions in Chapter 7 has shown that a minimum setpoint of $0.5 \text{ g O}_2/\text{m}^3$ is required to ensure acceptable robustness of effluent quality to influent perturbations, whilst solutions with a setpoint below $0.7 \text{ g O}_2/\text{m}^3$ typically provide unacceptable effluent quality reliability. In light of this, and the fact that

sufficient DO must be provided for nitrification, it is recommended that a minimum DO concentration of $0.7 \text{ g O}_2 / \text{m}^3$ is maintained, although a setpoint this low is not necessarily recommended – a range of options should be evaluated on a site-specific basis and one providing the required emission reduction with acceptable costs and effluent quality selected.

Carbon Source Addition

Analysis of optimised solutions providing a significant reduction in GHG emissions with no increase in operational costs has shown a decrease in external carbon source addition in the first anoxic reactor to be a common feature. Reducing carbon source addition is clearly desirable in that it reduces both GHG emissions and operational costs associated with production of the chemicals, and previous studies (Flores-Alsina et al. 2011, Stensel et al. 2013) have noted that adding external carbon increases GHG emissions. Flores-Alsina et al (2011) found that a low COD/N ratio, resulting from removal of all external carbon source addition, actually increased direct N_2O emissions due to incomplete denitrification; however, this was to a lesser degree than the reduction in emissions from biomass respiration and BOD oxidation which was also observed and it was concluded that “*in terms of GHG emissions it seems that it is better not to add carbon*”. Evidently, the impacts on effluent quality must be considered, however.

Optimal solutions in this research also contained low carbon source addition rates in the second anoxic reactor, however, suggesting that a complete removal of all external carbon may not provide the greatest benefits. Therefore, it is suggested that future control strategy development consider a reduction in carbon source addition but, if carbon addition is currently found to be necessary to achieve acceptable performance for the plant in question, it is not necessarily completely removed. Carbon source addition should not be increased since this has been shown to increase emissions resulting from biomass respiration and BOD oxidation, chemical production, and sludge processing and disposal (Flores-Alsina et al. 2011).

In this study, only static carbon source addition rates were considered – it may be that further improvement can be achieved with dynamic control to maintain a required minimum COD/N ratio.

Controller Tuning Parameters

Tuning parameters are a key factor in ensuring correct performance of WWTP control strategies, and are commonly adjusted on the basis of trial and error (Rojas et al. 2012). Suitable values will be case-specific, so detailed recommendations cannot be made. However, a common feature of optimised solutions providing a reduction in GHG emissions with no increase in operational costs (for the WWTP studied in Section 6.1) is an increase in the integral time constant of the PI controller. This suggests that a slow controller may be preferable and the effects of increasing the integral time controller (if a PI controller for DO control is already present) should be investigated.

8.3.2 Low Priority for Investigation

Sensitivity analysis is a useful tool for identification of key control handles affecting GHG emissions; however, it should not be assumed that all control handles to which GHG emissions are sensitive can be used to bring about improvements or are good candidates for optimisation.

For example, aeration intensities in the first activated sludge reactors, which are conventionally operated under anoxic conditions, were classified as highly sensitive based on GHG emissions in this research and thus included as decision variables for optimisation. Analysis of optimised solutions showed, however, that high aeration intensities correspond with poor effluent quality robustness to influent perturbations and that low or no aeration is preferable in terms of effluent total nitrogen reliability. Sensitivity analysis also showed operational costs to be sensitive to carbon source addition rates in the aerobic activated sludge reactors, where they would usually be zero, but optimised solutions in which external carbon was added here failed to provide reliable, robust and resilient design.

It is recommended that standard design rules and operating practices are observed and that changes such as aeration in 'anoxic' reactors and carbon source addition in aerobic reactors are not considered a priority for investigation. Whilst such changes may contribute to a heavily optimised solution which performs well under a specific set of conditions, they are likely to be detrimental to performance under future uncertainties and reduce robustness and resilience.

8.4 Control Strategy

There are many alternative WWTP control options which may be used to provide an improvement in effluent quality and/or reduction in costs, ranging from PI and cascade controllers to rule-based algorithms and model predictive control (Åmand et al. 2013). However, these may result in an inadvertent increase in GHG emissions; Guo et al. (2012a), for example, found ammonia-DO cascade control to cause problems with high N_2O emissions. It is important, therefore, that any change in control strategy is not implemented without detailed investigation into the effects on GHG emissions. It is also important to consider the effects of emission reduction measures on emissions from a range of different sources rather than focussing on just one high priority source. Increasing the SRT, for example, can result in net emission and cost reduction, despite increasing direct non- N_2O emissions.

It has been shown in Chapter 6 that appropriate DO control can have a significant impact on GHG emissions and may allow emissions to be reduced at no additional cost whilst retaining a high quality effluent. Two control strategies providing DO control were investigated: one with a single sensor and setpoint, and another with individual sensors, setpoints and actuators for each aerated activated sludge reactor. While both could be used to provide a significant reduction in emissions, it was found that independent control of aeration in each reactor was able to do so whilst maintaining a better effluent quality.

Control of the spatial distribution of DO concentrations is important as it impacts heavily on N_2O production, and it has been suggested that using a single DO setpoint is insufficient due to the unknown DO spatial profile (Guo et al. 2012b). Independent control of aeration in each aerated activated sludge reactor has also been found to result in lower GHG emissions than open loop control or alternatives such as ammonia-DO cascade control, both under current conditions and under future increased wet weather disturbances (Guo et al. 2012a). It is, therefore, recommended that this be considered in future control strategy development.

In Chapter 6, independent DO control was found to perform particularly well when using a low setpoint ($0.5 \text{ g O}_2/\text{m}^3$) in the final reactor, and Guo et al. (2012b) recommend a higher DO setpoint in the first aerobic reactor to reduce

N₂O production by AOB denitrification. Whilst a setpoint as low as 0.5 g O₂/m³ may not achieve adequate effluent quality reliability and robustness (as discussed in Section 8.3.1), it is suggested that use of reduced DO concentrations in the final aerated reactor are investigated.

It has also been shown that significant improvements can be achieved through better control of the SRT, by manipulation of wastage flow rates. Although such adjustments are typically made manually and this study only considered three fixed flow rates, based upon temperature, improved selection of wastage flow rates even on this limited basis can be beneficial. Automated SRT control is not widely used in practice and has not been included in this research; given the sensitivity of GHG emissions to wastage flow rate, and the implied sensitivity to SRT, however, automated control may be worth pursuing.

8.5 Optimisation and Detailed Design

This research has shown that multi-objective optimisation of WWTP operational parameters and tuning parameters using NSGA-II can significantly reduce GHG emissions whilst maintaining a compliant effluent and not increasing operational costs, without the need to modify the plant or control strategy layout. A range of Pareto optimal solutions can be developed, from which a decision maker is required to choose one for implementation. One factor for consideration here may be predicted performance under both design conditions and when subject to threats; whilst optimisation enables development of solutions which maintain a compliant effluent with a high degree of reliability, robustness and resilience, not all perform satisfactorily and further in-depth analysis, post-optimisation, is recommended.

8.5.1 Trade-offs for Consideration

Multi-objective optimisation results show that GHG emissions may be reduced with no loss in effluent quality, but this is likely to increase costs; if costs are not to be increased then emission reduction may incur an increase in effluent nitrogen and ammonia. Application of this observation to other scenarios evidently dependent on quality of the existing control – if no control strategies are currently employed (i.e. the plant is operated in an open loop configuration) or the control is poor, simultaneous improvement in GHG emissions, operational costs and effluent quality may be achievable.

Irrespective of the benchmark performance, it is noted that solutions predicted to provide the lowest emissions and costs under design conditions typically result in a poor effluent quality and exhibit relatively poor effluent quality reliability, robustness and/or resilience. To ensure a solution which performs well in reality when subject to threats, therefore, it may not be reasonable to implement solutions which appear to provide the greatest GHG emission reduction.

8.5.2 Performance Evaluation

For multi-objective optimisation using NSGA-II to be feasible, it is necessary that the performance of each solution can be evaluated quickly (i.e. in a matter of seconds). This means that it is unlikely to be possible to simulate model outputs over an entire year, or other extended design periods, due to the high computational demand, and modelling of performance over just a few weeks may have to suffice.

Results obtained in Chapters 6 and 7 show that use of two short evaluation periods for each solution – one summer week and one winter week – enables identification of a wide range of solutions on the GHG emission / effluent quality / operational cost Pareto front, including solutions which provide a significant reduction in GHG emissions. However, a high proportion of solutions provide unacceptable effluent quality reliability when the design requirements are for compliance over a longer period. It is therefore suggested that as long an evaluation period as is practical, given the computational demand of the specific model and number of model evaluations required, should be used, and this should incorporate both summer and winter conditions. If this period is shorter than that which is required to describe design conditions, reliability of the preferred solutions must be assessed post-optimisation.

An alternative approach is to sample key decision variables rather than using a genetic algorithm; whilst this does not provide a global optimisation, it does enable identification of improved solutions. Due to the reduced number of model evaluations required in this method (depending of the number of decision variables considered and sampling resolution), it is possible to undertake a more thorough evaluation of each solution. For example, an extended evaluation period may be used to ensure that solutions provide the required

reliability. For computationally demanding models where performance during a short period is not necessarily representative of behaviour under the required range of design conditions, this approach is preferable.

8.5.3 Constraints and Objectives

Optimisation objectives should include minimisation of GHG emissions, operational costs and effluent pollutant loading. Despite the CRC requiring reduction of emissions resulting from energy use only, it is important from an environmental perspective that solutions are optimised to reduce total GHG emissions, since it is shown in Chapter 6 that the change in energy use may be disproportionate to the change in total GHG emissions. It is also possible that solutions providing a reduction in total GHG emissions may increase those reported under the CRC, and thus would be overlooked if only energy related emissions were minimised.

For minimisation of effluent pollutant loading, a single index to represent effluent quality (such as the EQI implemented in BSM2 (Nopens et al. 2010)) is recommended, as it is shown that, for a fixed number of model evaluations, this achieves solutions with a similar or better effluent quality than when specific pollutant loadings are minimised individually. This is also better from a decision maker perspective since it is easier to visualise and compare results when only one effluent quality measure is used.

It is also important that appropriate constraints are applied in the optimisation, to ensure that optimised solutions adhere to the required standards. These should take into account the relevant legislative standards for effluent quality; however, it is suggested that the effluent quality constraints should be stricter than the requirements set for compliance since solutions which provide effluent concentrations near the regulatory limit when evaluated on a short term basis are shown to have poor reliability, robustness and/or resilience. This applies to the effluent total nitrogen constraint in particular, as solutions which fail to provide an acceptable level of effluent quality reliability, robustness or resilience in this research typically do so due to elevated nitrogen concentrations.

8.5.4 Decision Variables for Optimisation

Selection of decision variables can be guided by the results of this study (Section 8.3) or, preferably, a site specific sensitivity analysis. This enables

identification of both highly sensitive control handles for which there may be significant benefit of including in optimisation, and non-influential control handles which should not be included. It is important also that common sense prevails and good operating practice is considered in the selection of decision variables. For example, this research showed that key model outputs were sensitive to aeration intensities in the 'anoxic' activated sludge reactors and external carbon source addition in the final aerobic reactor and, as such, these were included as decision variables in multi-objective optimisation; however, these would not conventionally be applied and, indeed, solutions with high values fared badly in reliability, robustness and resilience analysis.

8.6 Model Limitations and Uncertainties

8.6.1 Greenhouse Gas Emission Modelling Limitations

The guidelines presented for control strategy development are based on the results of GHG emission modelling in this thesis. However, the model used omits some potentially significant sources of emissions due to a lack of reliable estimation techniques at the time of development, and the effects on these of implementing the design recommendations must be considered.

It is suggested in Section 8.3.1 that a reduction in aeration / DO setpoint may be beneficial, for example, but it is important that the possible effects on N₂O production pathways which were not modelled are explored. N₂O emission from AOB denitrification, which has lately been found to account for more than 33% of N₂O emitted (Guo 2014), was not modelled but it is known that the maximum rate of N₂O emission from AOB denitrification occurs in low DO conditions (Ni et al. 2013). It has been suggested that, to minimise such emissions, a minimum DO setpoint of at least 0.5 g O₂/m³ should be maintained (Zheng et al. 1994).

It is also observed that many of the optimised solutions with low GHG emissions in Section 6.1 have high effluent ammonia concentrations. However, this may correspond with high emission of not-modelled N₂O emissions since NH₄⁺ is the source of nitrogen for N₂O formation from AOB pathways. Models for N₂O emission from AOB denitrification do now exist (e.g. Mampaey et al. 2013) and these emissions should be modelled in future analyses.

For assessment of control options for a different plant, development of a site-specific model is necessary, and this should include modelling of GHG

emissions from all sources for which it is practical to do so. It is recognised that it is not possible to model every source of emissions and that there will still be omissions; however, the likely impact of any operational changes on these emission sources should still be considered in a non-quantitative manner.

8.6.2 Modelled Performance Uncertainties

The model used in this study, and indeed N₂O emission models in general, are subject to a high degree of uncertainty (e.g. Sweetapple et al. 2013), with existing models as of yet unable to accurately replicate field measurements (Law et al. 2012a, Ni et al. 2013, Sperandio et al. 2014). Both modelled GHG emissions and effluent quality are highly sensitive to parameters associated with modelling of nitrogen conversions (Sweetapple et al. 2013), and uncertainty analysis using the influential parameters identified in Chapter 4 is recommended for solutions under consideration. Monitoring of N₂O emissions both before and after full-scale implementation of any changes would also be beneficial given modelling uncertainties and omissions.

8.6.3 Future Uncertainties

Further analysis is required following optimisation, to identify any unintended consequences. For example, some optimised solutions have been shown to perform poorly with respect to reliability, robustness and resilience (Chapter 7), and it has previously been noted that optimisation can result in microbiology-related problems (Guerrero et al. 2012). If solutions are optimised using an evaluation period shorter than that required to cover the complete range of design and operating conditions, then assessment of effluent quality reliability is vital. Analysis of robustness and/or resilience is also recommended; however, it is recognised that these must be assessed with respect to a specific threat and it is not possible to consider all possible future uncertainties. As a minimum requirement, robustness of effluent total nitrogen to perturbations in temperature should be investigated since a reduction in temperature was found to be the most common cause of effluent quality failure in Section 7.4.

8.7 Guideline Summary

The following guidance is proposed:

1. Control strategies *MUST* be evaluated on a site specific basis – different WWTPs cannot be assumed to have the same response as

the plant under study in this research, although features found to contribute to a reduced emission solution here should be investigated.

2. Total GHG emissions should be minimised, not just those reported under the CRC. All emission sources for which it is practical to do so should be modelled, and the likely impact of changes on those not modelled must also be considered.
3. Site-specific sensitivity analysis can be used to guide selection of key control handles for adjustment, but standard design rules and operating practices should be observed. Use of control handles which are not conventionally employed may contribute to an improvement under very specific conditions but a decrease in robustness and resilience.
4. Selection of appropriate wastage flow rates is of key importance and automated SRT control, although not widely used, may be worth pursuing. High SRT solutions are preferable as these provide the greatest reduction in N₂O emissions, but be aware of problems such as low F/M bulking which can occur if wastage is insufficient.
5. Improved DO control may enable emission reduction at no additional cost whilst maintaining a high quality effluent. Controlling the spatial distribution of DO concentrations in activated sludge can be beneficial and independent control of aeration in each aerobic reactor should be investigated.
6. Reduction of DO setpoint may assist in reduction of GHG emissions, but sufficient DO must be maintained to prevent N₂O emissions associated with nitrification. Values of less than 0.7 g O₂/m³ are likely to result in incomplete nitrification and/or unsatisfactory effluent quality reliability and robustness.
7. If a PI controller is present for DO control, a slow controller may be preferable and effects of increasing the integral time constant should be analysed.
8. If an external carbon source is added to the first anoxic reactor, reduction or removal should be considered as this can reduce both GHG emissions and operational costs. If carbon source addition is unavoidable, dynamic control to maintain the required minimum COD/N ratio and improve efficiency could be considered.

9. All proposed changes should be implemented simultaneously in model evaluation as significant interaction effects between control handles have been identified.
10. A range of solutions providing emission reduction can be developed using multi-objective optimisation or sampling of key decision variables. If performance of a single solution cannot be adequately assessed within a matter of seconds then, from a computational demand perspective, the sampling approach is more preferable.
11. If the solutions are to be reliable, robust and resilient, effluent quality constraints applied in control strategy development / optimisation must be stricter than those required to achieve compliance. This applies particularly to the effluent total nitrogen limit.
12. If the evaluation period used in control strategy development / optimisation does not encompass the complete range of design conditions, analysis of reliability post-optimisation is recommended. In all cases, analysis of effluent quality robustness is recommended, in particular with respect to perturbations in temperature.

9 CONCLUSIONS AND RECOMMENDATIONS

9.1 Thesis Summary

Wastewater treatment results in significant emissions of GHGs and there is growing research interest in this area as a result of environmental concerns and tough emission reduction targets. Modelling of GHG production and emission from WWTPs is advancing and there has been investigation into factors affecting emissions. However, whilst there is emerging research into the potential benefits of improved WWTP control, there has been little previous work on control strategy optimisation for the reduction of GHG emissions, with no (identified) studies providing a detailed picture of the necessary trade-offs between GHG emissions, effluent quality and operational costs.

The aim of this research was to develop strategies for the reduction of GHG emissions from wastewater treatment processes, focussing on achieving optimal control of existing systems and reducing emissions resulting from their operation rather than developing new processes or recommending alternative treatment techniques.

To achieve this aim and in order to compare alternative strategies, it was first necessary to identify, develop or adapt a model which could be used. The literature review identified existing methods and models for quantifying GHG emissions, and appraised them with respect to their suitability for dynamic emissions modelling and control strategy assessment. As an appropriate comprehensive model was not available at this stage, existing emission estimation methodologies were implemented in the BSM2 to provide a basis for control strategy development.

Before using the model in optimisation, sensitivity analysis was carried out to identify key sources of uncertainty in the modelling of GHG emissions from wastewater treatment and provide a better understanding of WWTP model characterisation. By using both the one-factor-at-a-time method and a variance-based global sensitivity analysis method, critical parameters and parameter interactions which had not been considered in previous studies and could not be identified through one-factor-at-a-time sensitivity analysis alone were revealed.

The next stage of the research focussed on development and optimisation of control strategies to reduce GHG emissions whilst maintaining acceptable effluent quality and operational costs. To guide the selection of decision variables for optimisation and aid an efficient design process, sensitivity analysis of available control handles was undertaken. This enabled identification of control handles to which GHG emissions, effluent quality and/or operational costs are sensitive and for which dynamic control has the greatest potential benefits, taking into account both individual and interaction effects, and of trade-offs in performance measures resulting from adjustment of each control handle individually. Sources of GHG emissions with the greatest potential for reduction or severe adverse effects from adjustment of WWTP control were also identified by analysis of variance.

It was then shown that multi-objective optimisation of WWTP control using NSGA-II and three objectives (minimise GHG emissions, effluent pollutant loading and operational costs) can provide a significant reduction in GHG emissions without the need for plant redesign, and without increasing operational costs or effluent compliance failures. Trade-offs are necessary, however, and these were explored. Investigation into different strategies for dissolved oxygen control showed that implementation of an appropriate control strategy can also yield significant benefits in terms of GHG emissions, effluent quality and operational costs. Both total GHG emissions and emissions reported under the Carbon Reduction Commitment were evaluated for the optimised control strategies and the impact of minimising total GHG emissions on those that are reported was assessed.

A review of the concepts of reliability, robustness and resilience definitions was carried out and different views analysed. Following selection of appropriate definitions and measures for application to WWTP control strategies, further analysis was undertaken to investigate the impact of optimisation to minimise GHG emissions on the reliability, robustness and resilience of control strategies. These were assessed with respect to both GHG emissions and effluent compliance, and threats/disturbances considered included sensor failures and various influent perturbations. Solutions providing acceptable performance under future uncertainties were compared with those providing unacceptable

performance and control features which contribute to a more desirable solution were identified.

Lastly, guidelines for the development of WWTP control strategies to reduce GHG emissions in a cost effective manner whilst maintaining an acceptable effluent quality were developed. There are based upon the results presented in Chapters 5-7 and take into the account robustness and resilience of control options as well as performance under design conditions.

9.2 Conclusions

The main conclusions reached with respect to each of the research objectives are summarised in the following sections.

9.2.1 *Assessment of Greenhouse Gas Emissions from Wastewater Treatment under Dynamic Loading*

Chapters 2, 3 and 4 addressed the background research required for quantification of GHG emissions, development of a model for assessment of direct and indirect operational GHG emissions under dynamic loading in addition to performance with respect to treatment standards, and analysis of this model to identify key sources of uncertainty and guide future work. Key conclusions drawn include:

- Modelling and quantification of dynamic GHG emissions poses many challenges and some emission sources, such as stripping of CH₄ formed in the sewer system and CH₄ resulting from unintentionally anaerobic conditions, are typically omitted due to a lack of reliable estimation methods. Empirical formulae should be avoided where possible for direct emissions if the model is to be used for comparing control strategies.
- An emissions model was developed which enables assessment of dynamic emissions under different control options. This is not comprehensive, however, with sources for which no suitable model was available not included. In particular, the effects of emission reduction measures on N₂O from nitrifier denitrification, which is not modelled, must be considered, as uncertainty in total GHG emissions results primarily from uncertainty in direct N₂O emissions due to their high GWP.
- Calibration of parameters used in modelling of nitrogen conversions is especially important since they are key sources of uncertainty in both

effluent quality and GHG emissions. Interaction effects as well as individual effects are significant and in future analysis it is important that a GSA method that enables identification of these is used.

- Recent advances have improved modelling of N₂O emissions but have not been included in assessment of GHG emissions in this research as they were published after completion of the model development stage.

9.2.2 Development and Optimisation of Control Strategies to Reduce Greenhouse Gas Emissions

Control strategy development was guided by sensitivity analysis for identification of sensitive emission sources and key control handles (Chapter 5), followed by optimisation using NSGA-II and decision variable sampling (Chapter 6). Important findings from these chapters are as follows:

- Adjusting a single control handle can result in a small change in effluent quality and/or operational costs but a significant change in GHG emissions. Therefore, it is vital that the effect on GHG emissions is considered in attempts to improve effluent quality and/or reduce costs.
- Multi-objective optimisation of key operational parameters and controller tuning parameters may enable a reduction in GHG emissions without alteration to the wastewater treatment processes employed and with no additional operational costs. However, if costs are not increased, this is likely to result in increased effluent nitrogen and ammonia concentrations. For effective optimisation, it is preferable to include minimisation of pollutant loading as an objective function, with pollutant loading represented by a single effluent quality index.
- Selection of a suitable aeration intensity in the final tank and wastage flow rate in the activated sludge unit is of key importance. Significant improvement in GHG emissions can be achieved with better control of wastage flow rates alone, but the effects on effluent quality and operational costs, which may also be significant, must be considered. Independent control of aeration in each activated sludge reactor, with a low DO setpoint in the final reactor, may also contribute to a reduction in both GHG emissions and operational costs whilst maintaining a high effluent quality.

- The emission source with greatest scope for improvement, and from which it is particularly important to ensure that emissions are monitored, is N₂O from the activated sludge process. However, the effects of emission reduction measures on total emissions must be considered since a reduction in N₂O emissions can correspond with an increase in non-N₂O emissions (although the net effect may still be favourable).

9.2.3 Analysis of Impact of Reducing Total Greenhouse Gas Emissions on Reported Emissions

The effects of control strategy development and optimisation to reduce total GHG emissions on emissions which companies are compelled to report under the CRC (i.e. those associated with net energy use in the WWTP) were analysed in Chapter 6. It was concluded that:

- Optimised solutions which provide the greatest reduction in total GHG emissions typically also reduce emissions reported under the CRC. However, for solutions which retain a high effluent quality, the percentage reduction in reported emissions is significantly less than that in total GHG emissions, suggesting that design to improve GHG emissions under the CRC alone will not yield the maximum potential environmental benefits.
- Solutions with the greatest energy recovery do not necessarily perform best with respect to reduction in total GHG emissions.
- In some instances, total GHG emissions may be reduced significantly whilst retaining a high quality effluent but increasing emissions associated with energy use; such solutions are disincentivised under the CRC but may be environmentally beneficial.

9.2.4 Investigation into Reliability, Robustness and Resilience of Optimised Control Strategies

Chapter 7 investigated the impact of optimisation on effluent quality and GHG emission reliability, robustness to influent perturbations and resilience to sensor failures. Features which correspond with poor reliability, robustness and resilience were also explored and many of the findings fed into the control strategy guideline development objective. The main findings include:

- Further analysis of solutions following optimisation is important to ensure those chosen perform as required when subjected to threats, as not all solutions which perform as required under the conditions used for performance assessment in the optimisation process are reliable, robust and resilient. However, it is possible to identify solutions which provide significant emission reduction whilst retaining a high degree of reliability, robustness and resilience (with respect to the threats considered in this research).
- Elevated nitrogen concentrations are a key source of failure in solutions which provide unacceptable effluent quality reliability, robustness or resilience, so control strategies should be designed to provide an effluent nitrogen concentration significantly better than that required for compliance.
- Unconventional practices such as low levels of aeration in ‘anoxic’ activated sludge reactors and external carbon source addition in aerated reactors may occur in optimised solutions and perform well under design conditions, but are likely to result in unacceptable effluent quality robustness and resilience.

9.2.5 *Development of Guidelines for Wastewater Treatment Plant Operation to Reduce Greenhouse Gas Emissions*

A set of guidelines for WWTP operation and control strategy development was produced in Chapter 8. To inform the guidelines, control strategy features that contribute to a reduction in GHG emissions were explored in Chapter 6, with those that do so whilst retaining an acceptable degree of reliability, robustness and resilience identified in Chapter 7. Results presented in Chapters 4 and 5, regarding key sources of uncertainty, sensitive emission sources and key control handles for emission reduction were also taken into account. The guidelines cover five key topics: GHG emission sources, key control handles and decision variables, choice of control strategy, optimisation and detailed design, and model limitations and uncertainties. Specific guidelines are not repeated here as they are based largely on the conclusions listed in Sections 9.2.1 - 9.2.4. However, key observations and recommendations which have not already been discussed in this chapter include:

- Emission reductions can be achieved with both high wastage flow rate (low SRT) and low wastage flow rate (high SRT) solutions. However, the high SRT solutions result in greater decrease in N₂O emissions from activated sludge, which is a preferable scenario given the significant uncertainty in N₂O emission modelling. These solutions are also able to provide a high quality effluent.
- Solutions providing a significant N₂O emission reduction using a high SRT may increase energy use and thus be undesirable under the CRC.
- It is important that the effects of changes in DO control and aeration are assessed in conjunction with any other modifications made (e.g. adjustment of wastage flow rate), as aeration intensities are involved in significant interaction effects.
- A low DO setpoint in the final activated sludge reactor can contribute to a reduction in GHG emissions; however, sufficient DO must be maintained for nitrification and too low a setpoint will reduce effluent quality robustness to influent perturbations and resilience to sensor failure.
- Carbon source addition should not be increased, and should be avoided entirely if possible, as it contributes to GHG emissions from multiple sources.
- If multi-objective optimisation is used for control strategy development, it may not be sensible to implement solutions which appear to provide the greatest emission reduction as they may perform poorly in reality when subject to threats (further analysis is required to assess performance under uncertain future conditions).
- Control strategies developed in this research may be less desirable with respect to total GHG emissions reduction than anticipated when all emission sources, including those not modelled, are considered. In particular, it is important that the likely effects of changes on N₂O emissions from AOB denitrification are considered. If possible, these should be included in future modelling and monitoring of N₂O emissions both before and after full-scale implementation of any changes would be beneficial.

9.3 Recommendations for Further Research

A number of potential topics for future research which follow on from the work presented in this thesis have been identified. In particular, further work which investigates the impact of suggested emission reduction measures on emissions from sources not modelled in this study and, if necessary, explores new strategies which could provide greater overall benefits, is recommended. Additional areas of research which could be explored include the impacts of control optimisation on a wider range of risks and failure modes, physical testing of control strategies in pilot scale and/or full scale experiments, and the potential of control at an integrated urban wastewater system level to provide greater emission reduction. These suggestions are discussed in more detail below.

9.3.1 Investigation into the Effects of Suggested Emission Reduction Measures on Emissions from Sources Not Modelled

A number of possible emission sources were omitted from the model detailed in Chapter 3 and used for control strategy development/optimisation and guideline development, due to a lack of reliable estimation techniques. These include direct CH_4 emissions resulting from poorly managed treatment and unintentionally anaerobic conditions, and N_2O emissions associated with nitrifier denitrification by AOB during nitrification.

As N_2O emissions have already been shown in this thesis to be a major contributor to uncertainty in modelled GHG emissions, it is particularly important that further research investigates the effects of proposed emission reduction measures on N_2O from alternative production pathways. It also has been suggested that nitrifier denitrification by AOB, rather than heterotrophic denitrification, is the main contributor to N_2O emissions (Law et al. 2012b), emphasising the importance of further work in this area.

There have recently been significant advances in the modelling of N_2O emissions, with extensions developed for the existing activated sludge models ASM1 (ASMG1) (Guo and Vanrolleghem 2014) and ASM2d (ASMG2d) (Guo 2014) which incorporate N_2O production from both heterotrophic denitrification and nitrifier denitrification by AOB. These have not been included in this thesis as they were published after completion of the model development stage of the

work. For future work, however, it is recommended that use of alternative models is considered. In particular, the latest BSM2G (Flores-Alsina et al. 2014), which incorporates ASMG1, provides a more complete description of emissions resulting from wastewater treatment than the earlier model version detailed by Flores-Alsina et al. (2011) and discussed in Sections 2.2.1-2.2.6. Use of this for future work rather than the model developed in this thesis would enable a more complete assessment of GHG emissions (since it includes modelling of N_2O from nitrification, which is a significant omission in this work). It would also enable benchmarking of control strategies against those from other research and would facilitate wider application of research findings.

Further sensitivity analysis of the available control handles using this model may enable identification of additional control handles to which total GHG emissions are sensitive, providing new avenues for exploration in control strategy development, or alter the priorities and focus of emission reduction measures. Use of a more inclusive but more complex model would also increase the potential sources of uncertainty, however, and further investigation to assess the effects on overall uncertainty in modelled GHG emissions and other performance measures would be recommended.

9.3.2 *Risks and Alternative Failure Modes and Performance Measures*

In this thesis, WWTP performance was assessed based on effluent quality, operational costs and GHG emissions only; potential problems such as those relating to biomass separation could not be modelled and were not, therefore, considered. However, it is possible that some of the optimised solutions would result in problematic behaviour if implemented in practice – for example, filamentous bulking may occur when DO in the aerated tanks is low, and uncontrolled denitrification in the secondary settler may cause rising sludge.

Further work should investigate the impact of control strategy optimisation on the risk of various performance problems including, but not limited to, filamentous bulking, filamentous foaming and rising sludge, and aim to determine the additional constraints required to produce solutions with an acceptably low risk. A risk assessment module exists for BSM2 (Dalmau et al. 2008) and could be used as the basis for further work. However, in its current

form, it is likely to be impractical to include in the performance assessment process during multi-objective optimisation due to its computational demand.

9.3.3 Pilot Scale and/or Full Scale Experiments

Calibration difficulties and the inability of some GHG emission models to accurately and consistently predict emissions from real WWTPs under dynamic loading have been noted previously (e.g. Law et al. 2012a, Ni et al. 2013, Sperandio et al. 2014). Models are also typically calibrated using data collected under 'normal' control of the plant; however, if model-based optimisation yields solutions with significantly altered control (particularly if the suggested control strategy is unusual), this may result in the plant operating outside the range for which it has been calibrated. In such a case, it may not perform as well in practice as expected based on the results of modelling.

Physical modelling of alternative control strategies, either at a pilot scale initially or at full scale, would be greatly beneficial. Dynamic emission data could be used to assess the accuracy of the model used for optimisation and ensure that implementing optimised control strategies achieves the desired effect. Alternatively, if recorded performance bears a poor resemblance to that modelled, good quality data will be necessary to guide the development of improved models and calibration. Of particular importance is monitoring of N₂O emissions, since production of this gas is the greatest source of uncertainty in modelled emissions as well as the source with greatest scope for improvement. Further work on an alternative plant, with either modelling or physical experiments, is also recommended for evaluation of the guidelines developed in Chapter 8.

9.3.4 Investigation into Potential Benefits of Control on an Integrated Urban Wastewater System Level

There is scope for further research on development of alternative control strategies for GHG emission reduction, including at an urban wastewater system level. Use of both feed-back control and feed-forward control (utilising, for example, river water quality and rainfall measurements) could be explored, as it was only possible to evaluate a limited number of control strategies in this thesis.

It is anticipated that control strategies which use data from an entire catchment, covering the sewer system, WWTP and receiving water body, will enable increased reduction in energy use and associated GHG emissions. If modelling the entire urban wastewater system, it is also recommended that CH₄ formation in sewers and means by which formation and/or stripping on entry to the WWTP can be reduced are investigated.

APPENDICES

Appendix A: Calculation of One-Factor-at-a-Time Sensitivity Indices for Wastewater Line and Sludge Line Emissions

OAT sensitivity indices represent the change in wastewater line and sludge line GHG emissions resulting from variation of individual control handles, as a percentage of base case total GHG emissions, and are calculated as follows. *WW* denotes wastewater line, *S* denotes sludge line, *i* denotes control handle number, *base* denotes base case, *upper* denotes output corresponding to the control handle upper bound value and *lower* denotes output corresponding to the control handle lower bound value.

$$E_{total,base} = f(x_{1,base...n,base}) \quad \text{Eq. A.1}$$

$$E_{WW,base} = f(x_{1,base...n,base}) \quad \text{Eq. A.2}$$

$$E_{S,base} = f(x_{1,base...n,base}) \quad \text{Eq. A.3}$$

$$E_{WW,i,upper} = f(x_{i,max}, x_{\sim i,base}) \quad \text{Eq. A.4}$$

$$E_{WW,i,lower} = f(x_{i,min}, x_{\sim i,base}) \quad \text{Eq. A.5}$$

$$E_{S,i,upper} = f(x_{i,max}, x_{\sim i,base}) \quad \text{Eq. A.6}$$

$$E_{S,i,lower} = f(x_{i,min}, x_{\sim i,base}) \quad \text{Eq. A.7}$$

$$P_{WW,i,upper} = 100 \times \frac{E_{WW,i,upper} - E_{WW,base}}{E_{base}} \quad \text{Eq. A.8}$$

$$P_{WW,i,lower} = 100 \times \frac{E_{WW,i,lower} - E_{WW,base}}{E_{base}} \quad \text{Eq. A.9}$$

$$P_{S,i,upper} = 100 \times \frac{E_{S,i,upper} - E_{S,base}}{E_{base}} \quad \text{Eq. A.10}$$

$$P_{S,i,lower} = 100 \times \frac{E_{S,i,lower} - E_{S,base}}{E_{base}} \quad \text{Eq. A.11}$$

where:

E = GHG emissions

x = control handle value

n = number of control handles

$x_{\sim i}$ = value of all control handles except x_i

P = Percentage change (OAT sensitivity index)

Appendix B: Multi-Objective Optimisation Convergence

Performance of solutions from different generations of the optimisation process are compared and analysed to ensure that sufficient generations are carried out to achieve an acceptable level of convergence; in the final generations, further significant improvements in the Pareto front should not be observed.

Online convergence analysis may be carried out to provide termination criteria. For example, the optimisation may be terminated once the improvements measured during a specified period fall below a threshold value. Alternatively, maximum number of generations or maximum execution time are simpler, more commonly used termination criteria (Trautmann et al. 2008). In this study, a maximum number of generations is specified and offline convergence analysis performed to ensure the value selected is sufficient.

Convergence is assessed using the metric of Deb and Jain (2002). This requires knowledge of a target (reference) set of points; in this instance, all non-dominated solutions from a 50 generation optimisation run are used as the reference set. The convergence metric (C) is the normalised average distance from nearest point in the target set (\mathbf{P}^*) for all solutions in generation analysed, calculated as follows (Deb and Jain 2002):

1. Identify set of non-dominated solutions, $\mathbf{F}^{(t)}$, from population for generation t , $\mathbf{P}^{(t)}$.
2. Calculate smallest, normalised Euclidean distance (d) to \mathbf{P}^* for each point (i) in $\mathbf{F}^{(t)}$ using Eq. A.12:

$$d_i = \min_{j=1}^{|\mathbf{P}^*|} \sqrt{\sum_{k=1}^M \left(\frac{f_k(i) - f_k(j)}{f_k^{max} - f_k^{min}} \right)^2} \quad \text{Eq. A.12}$$

where:

- $|\mathbf{P}^*|$ = Number of solutions in reference set
- j = Solution number in reference set
- M = Number of objectives
- k = Objective number
- f_k^{max} = Maximum value of k -th objective function in \mathbf{P}^*

f_k^{min} = Minimum value of k -th objective function in \mathbf{P}^*

3. Calculate convergence metric for generation t :

$$C(\mathbf{P}^{(t)}) = \frac{\sum_{i=1}^{|\mathbf{F}^{(t)}|} d_i}{|\mathbf{F}^{(t)}|} \quad \text{Eq. A.13}$$

4. Normalise $C(\mathbf{P}^{(t)})$ values as follows:

$$\bar{C}(\mathbf{P}^{(t)}) = \frac{C(\mathbf{P}^{(t)})}{\max(C(\mathbf{P}^{(t)}))} \quad \text{Eq. A.14}$$

Convergence for generations 1-25 of an optimisation using objective set X is shown in Figure A.1. Improvement slows beyond 20 generations and the convergence metric appears to begin to plateau. This suggests that further increase in the number of generations would be inefficient. Solutions from the final generations of the optimisation run using objective set X are presented in Figure A.2, which confirms that improvement in the position of the Pareto front is small as the number of generations approaches 25. There is also little change in the completeness of the Pareto front / spread of solutions and the shape of the Pareto front is consistent, suggesting it can reliably be used for identification of trade-offs. Given the high computational demand of the model, therefore, it is concluded that 25 generations are sufficient.

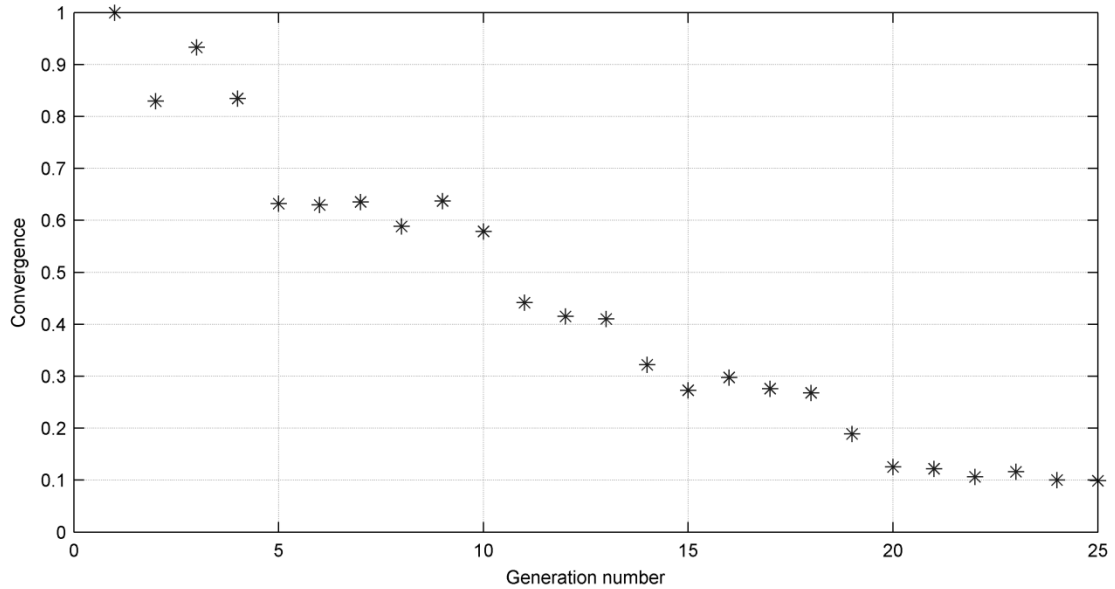


Figure A.1: Objective set X convergence

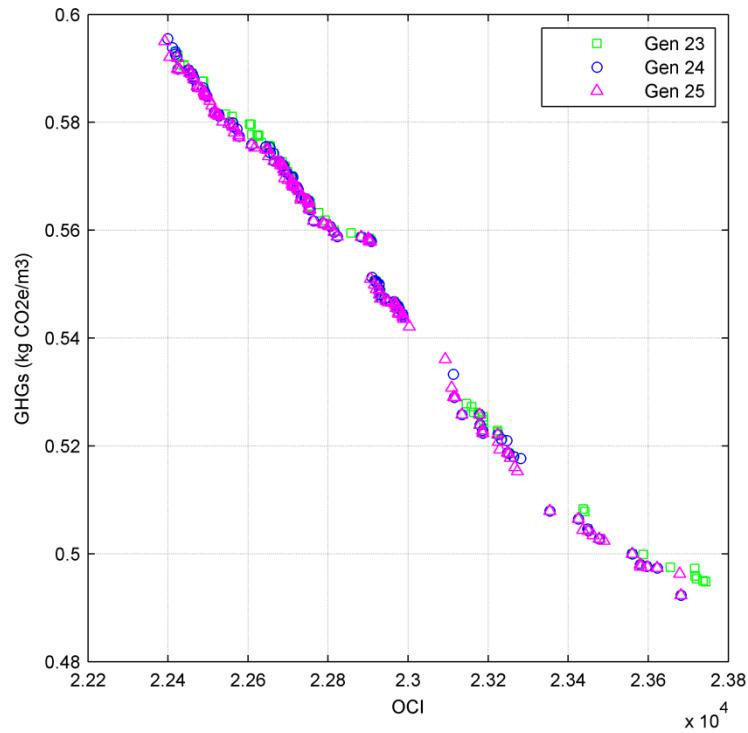


Figure A.2: Comparison of non-dominated solutions in final generations of optimisation run with objective set X

For evaluation of the preferred objective set for optimisation of control strategies to reduce GHG emissions, it is desirable that the same number of generations (and, therefore, model evaluations) is used for each objective set so that there is no significant change in computational demand. It is expected that an increase in objective functions would require an increased number of evaluations to reach the same level of convergence; however, given the high computational demand of the model, this would reduce the feasibility of the optimisation. To enable comparison of each objective set on a like-for-like basis, therefore, 25 generations are used in each case.

Despite not reaching the same level of convergence as objective set X, objective sets Y and Z produce acceptable performance with 25 generations. Convergence of a single optimisation run with each objective set is shown in Figure A.3, and solutions from the final three generations are presented in Figure A.4 and Figure A.5. For clarity, all results are presented using pair-wise comparisons of the trade-offs between each objective and only solutions which are non-dominated based on the two-objectives presented are shown in each plot.

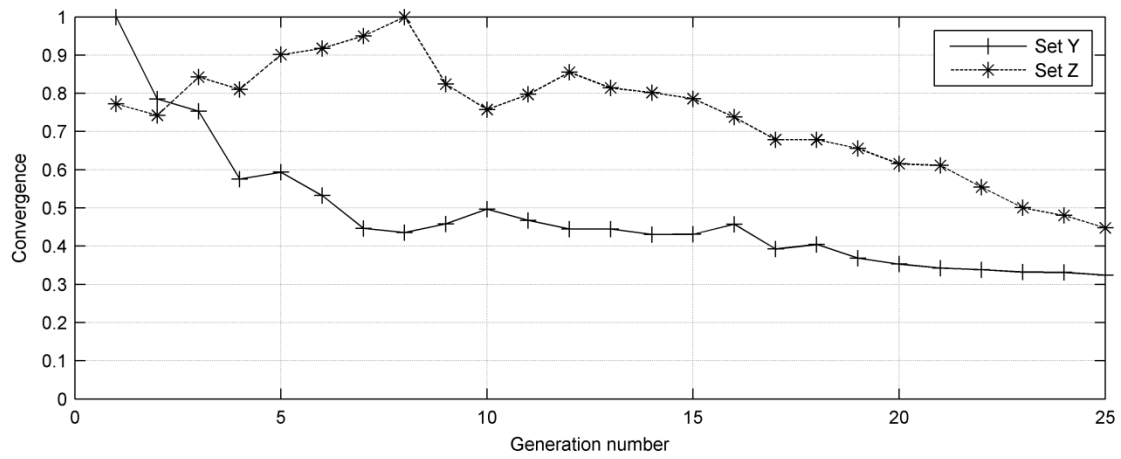


Figure A.3: Objective sets Y and Z convergence

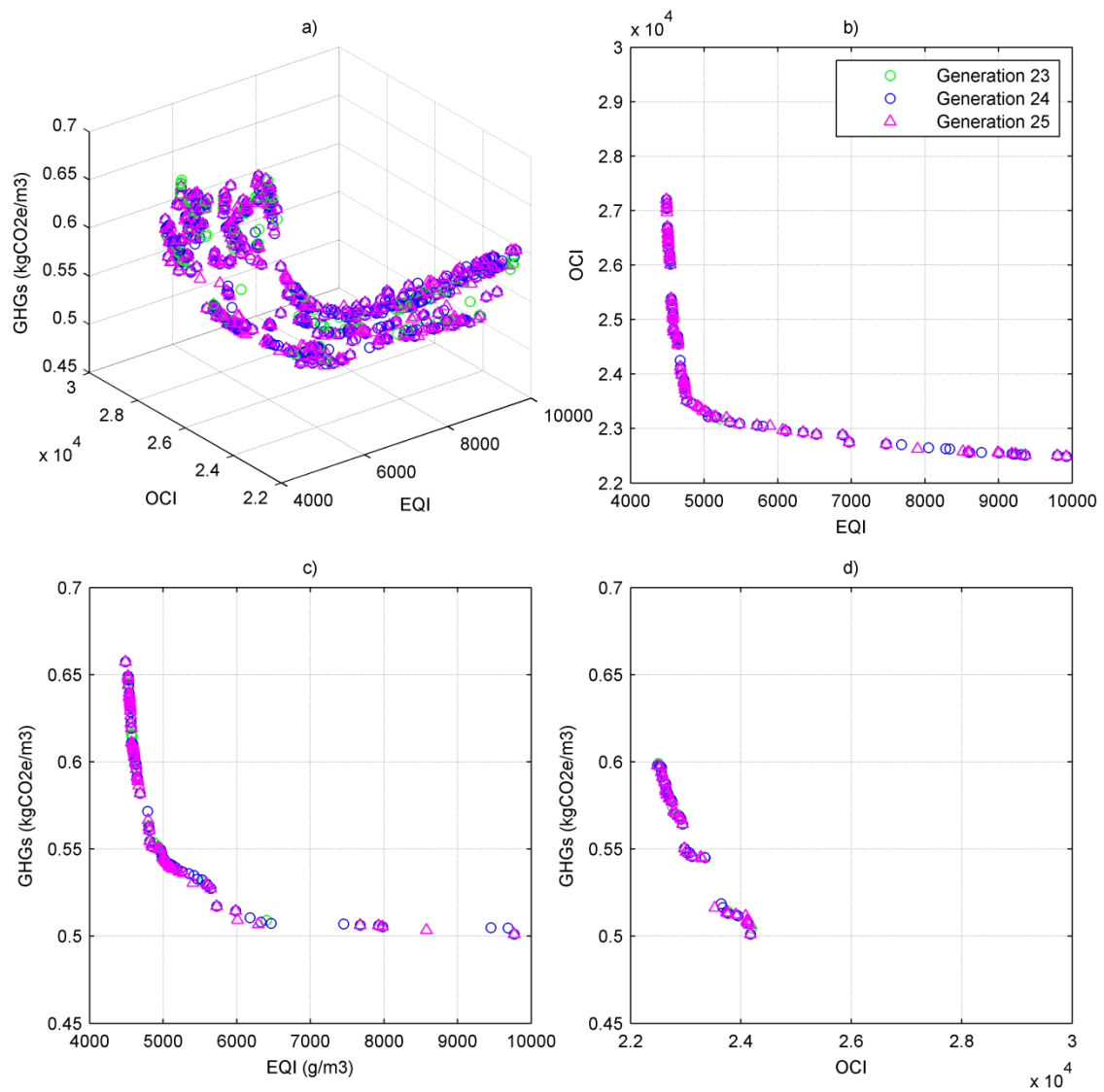


Figure A.4: Comparison of non-dominated solutions in final generations of optimisation run with objective set Y

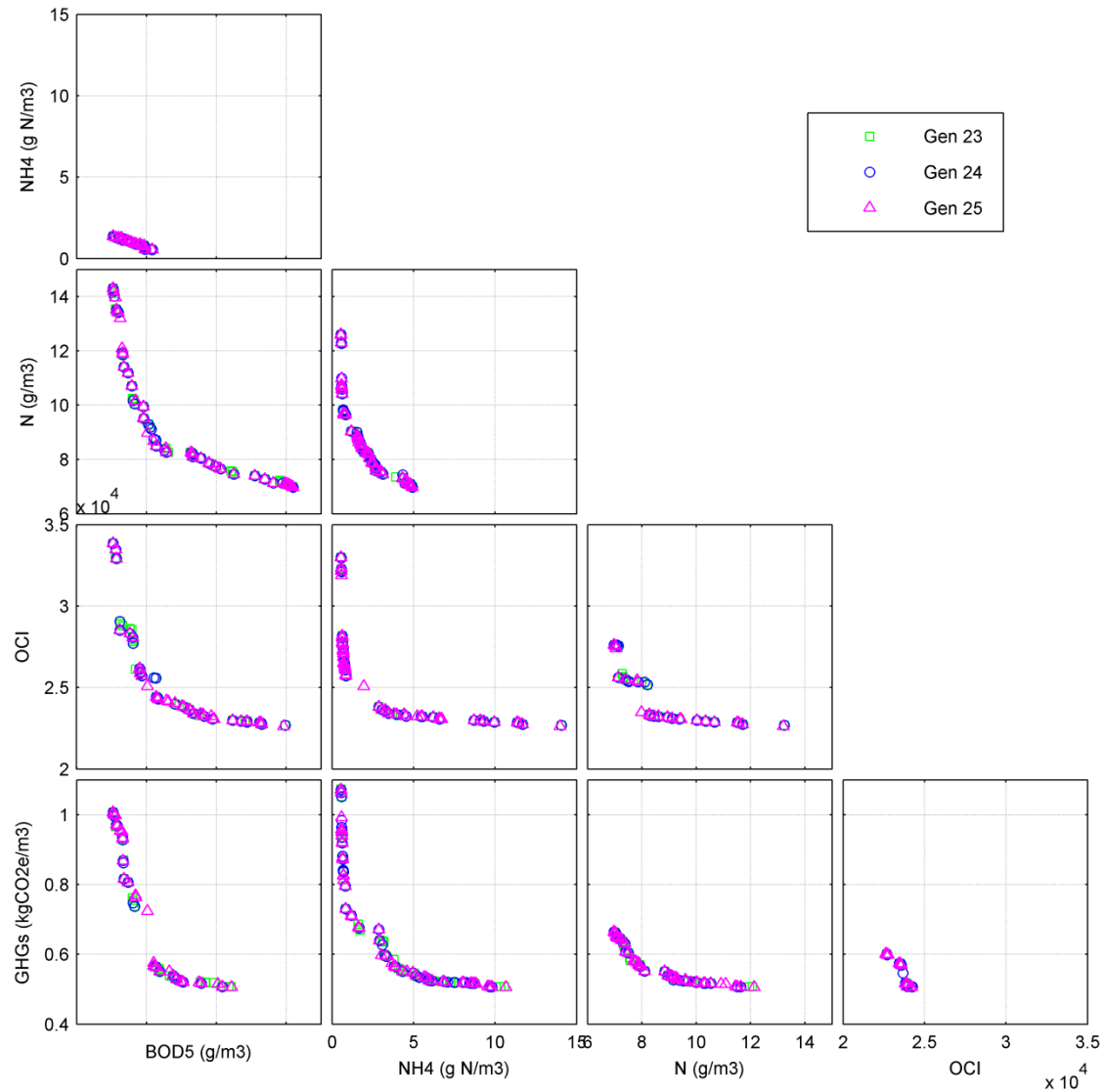


Figure A.5: Comparison of non-dominated solutions in final generations of optimisation run with objective set Z

Figure A.3 confirms that objective sets Y and Z reach a poorer level of convergence than set X within 25 generations, as expected due to the increased number of objectives. For objective set Y in particular, however, the increase in convergence observed with each additional generation towards the end of the optimisation run is small, and the additional number of generations (and, therefore, computational demand) required to achieve significant improvement in convergence would be substantial and impractical. Figure A.4 and Figure A.5 show that, despite the convergence indicators being relatively poor, little improvement in the position of the Pareto front is observed from generations 23 to 25 for either objective set, supporting the notion that further increase in the number of generations would be inefficient and likely to reap

little benefit without substantial additional computational cost. Therefore, it is concluded that, although increasing the number of generations above 25 would improve the final solutions, 25 generations provide a reasonable compromise between optimality of solutions and computational demand.

Appendix C: Performance of Control Strategies under Extended Performance Evaluation – Complete Results

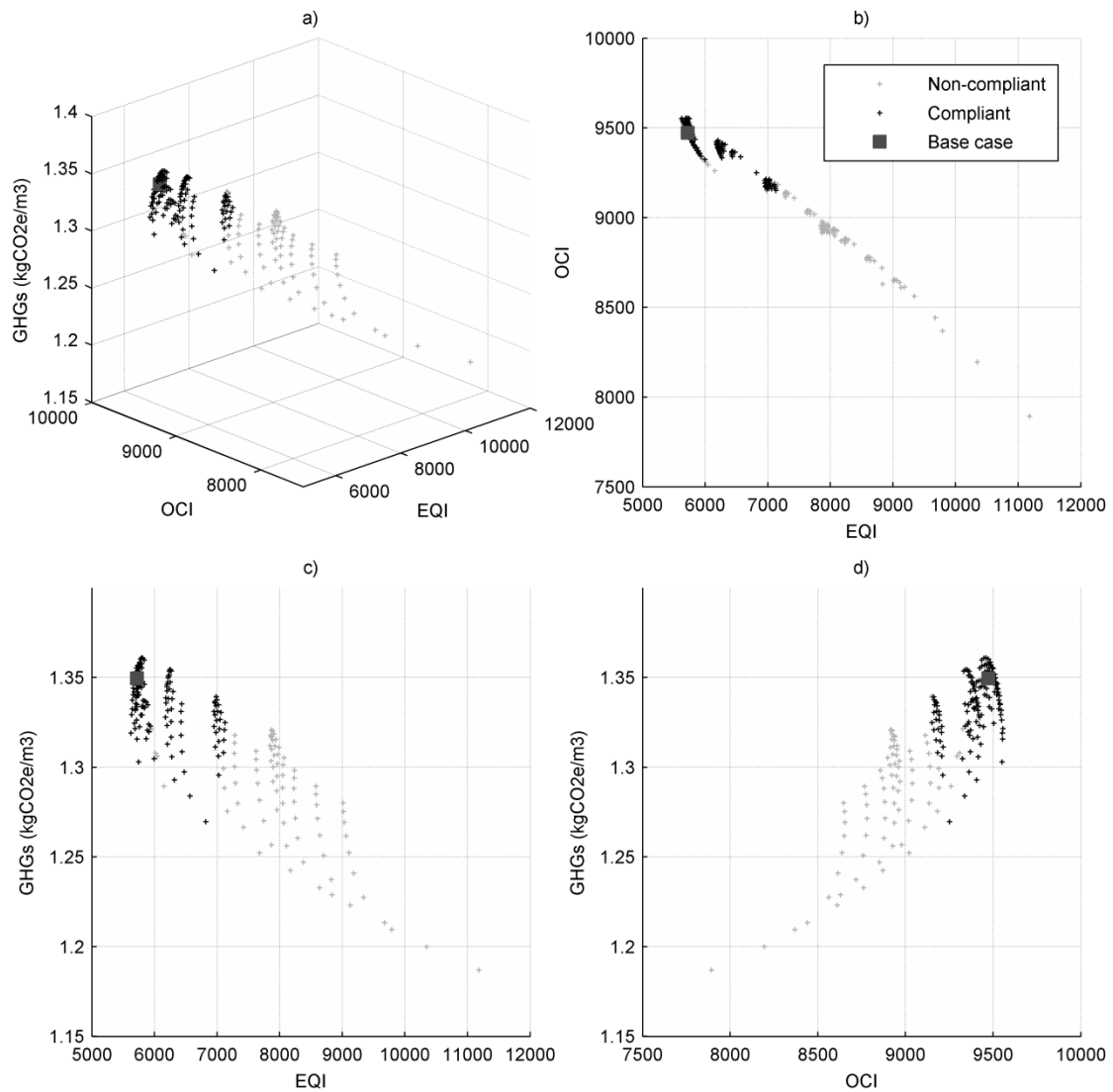


Figure A.6: WWTP performance with adjusted wastage flow rates in the DCL control strategy (compliant and non-compliant solutions)

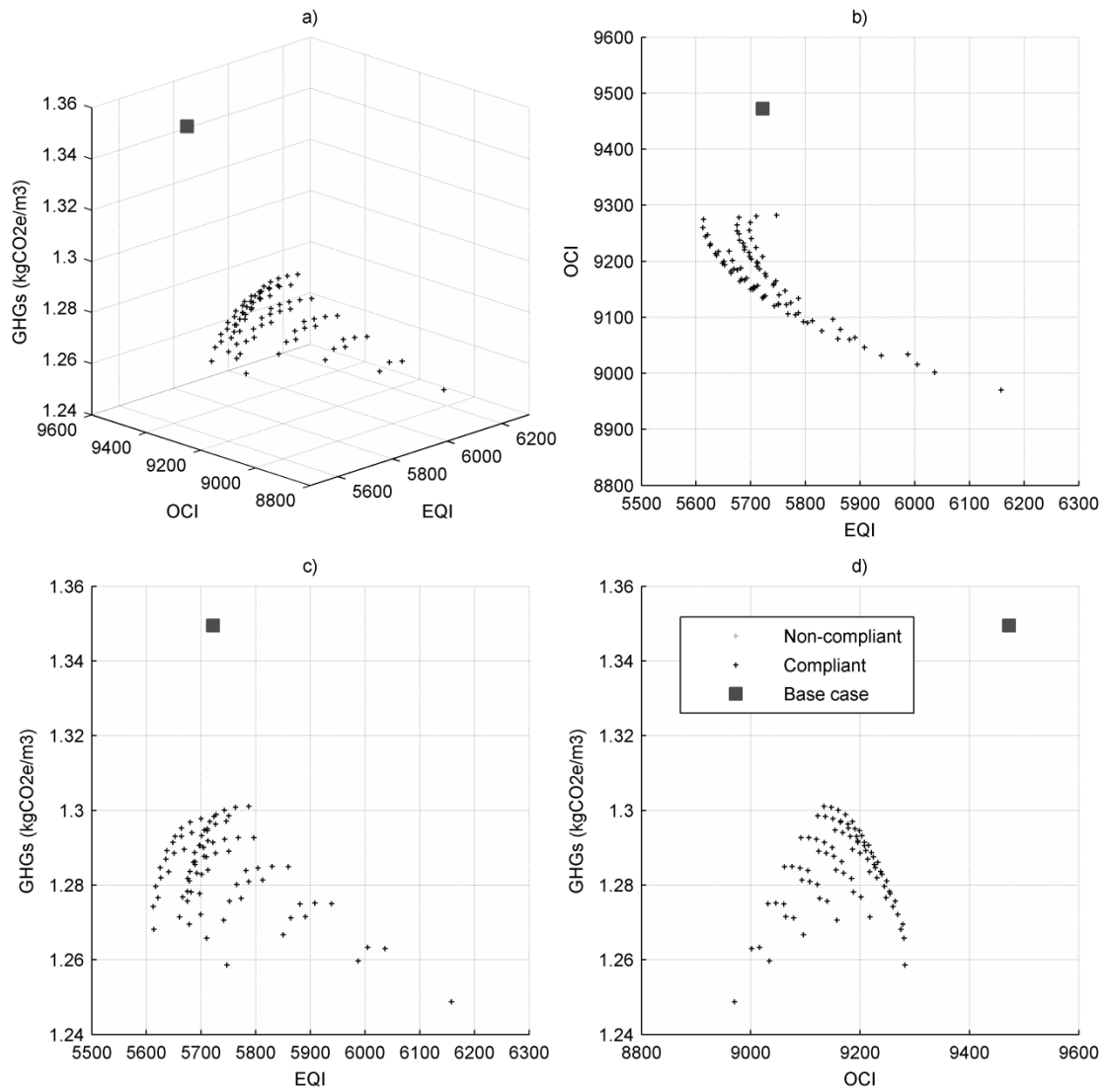


Figure A.7: WWTP performance with adjusted wastage flow rates in the 3-DO control strategy (compliant and non-compliant solutions)

Appendix D: Reliability Study – Complete Results

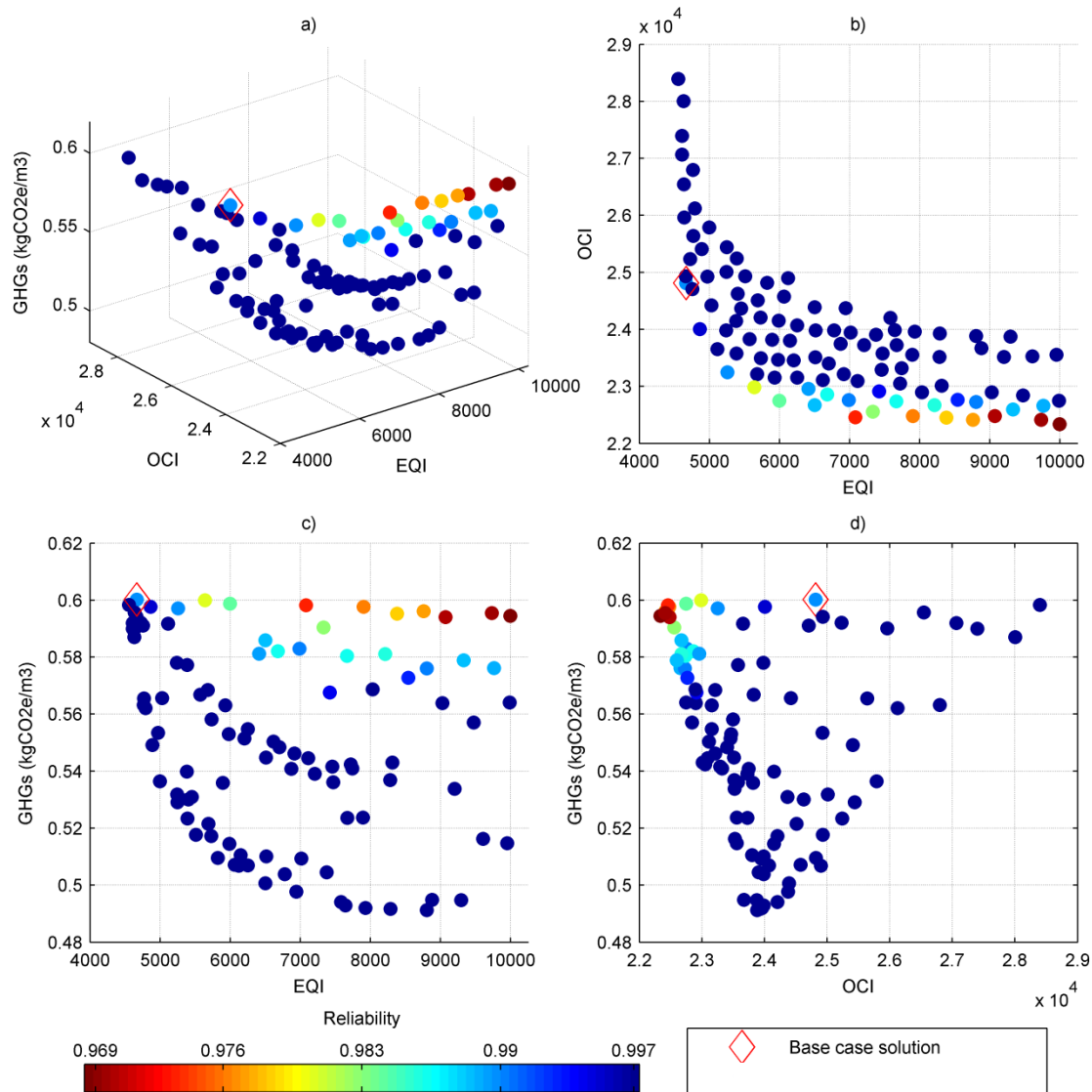


Figure A.8: Effluent BOD₅ reliability of non-dominated solutions bettering base case GHG emissions under default conditions

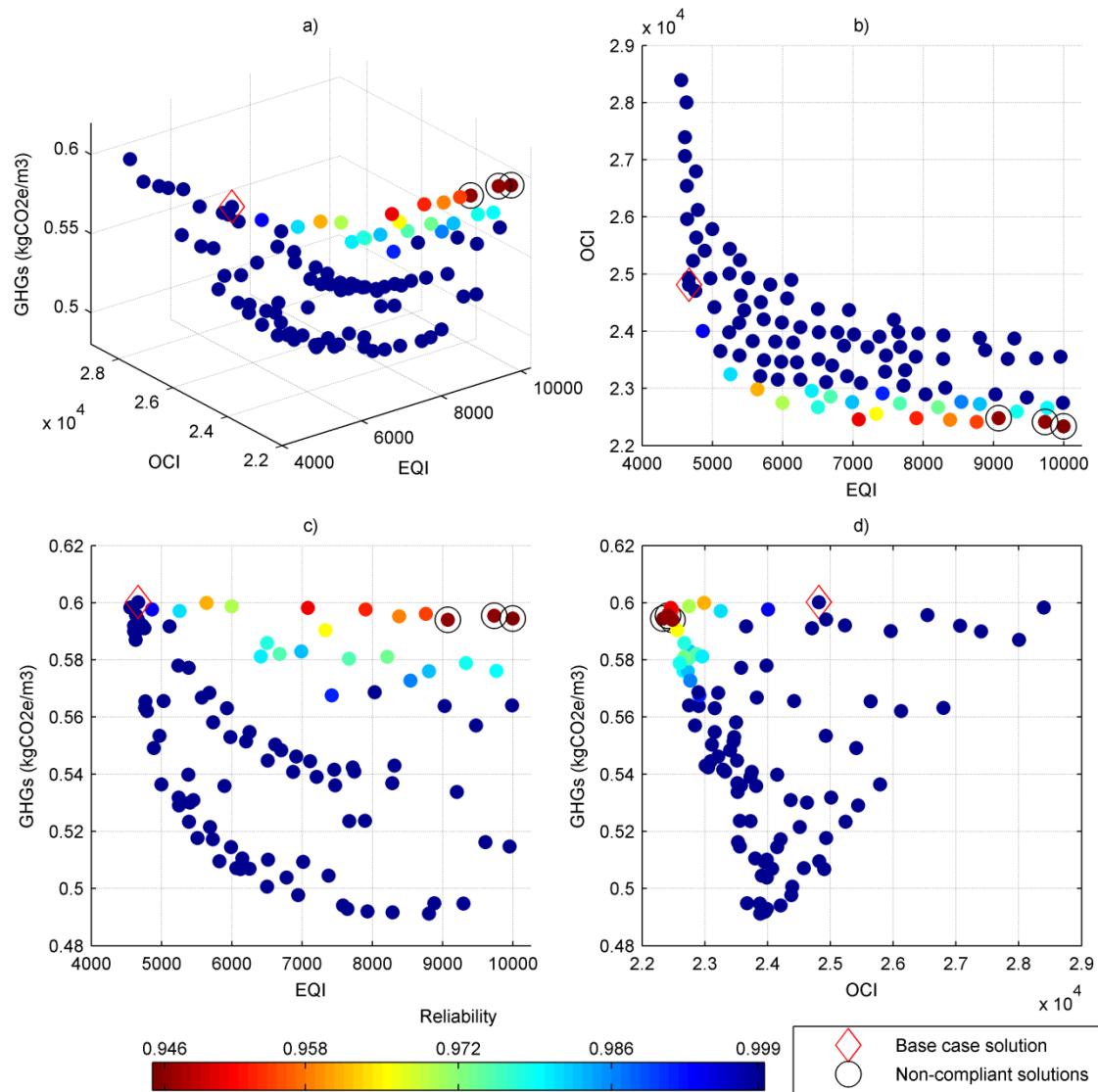


Figure A.9: Effluent COD reliability of non-dominated solutions bettering base case GHG emissions under default conditions, with solutions failing to achieve 95% compliance identified

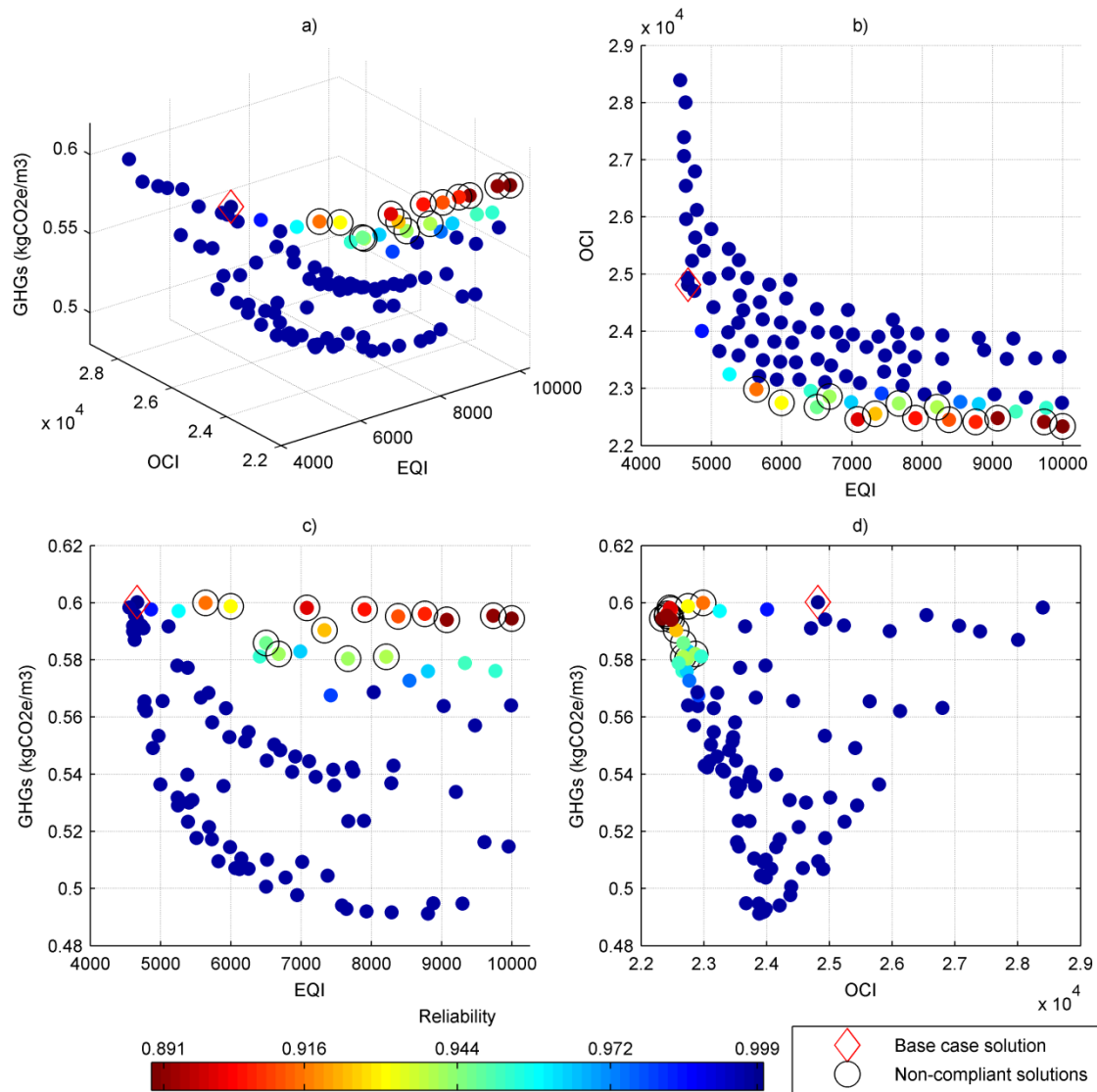


Figure A.10: Effluent TSS reliability of non-dominated solutions bettering base case GHG emissions under default conditions, with solutions failing to achieve 95% compliance identified

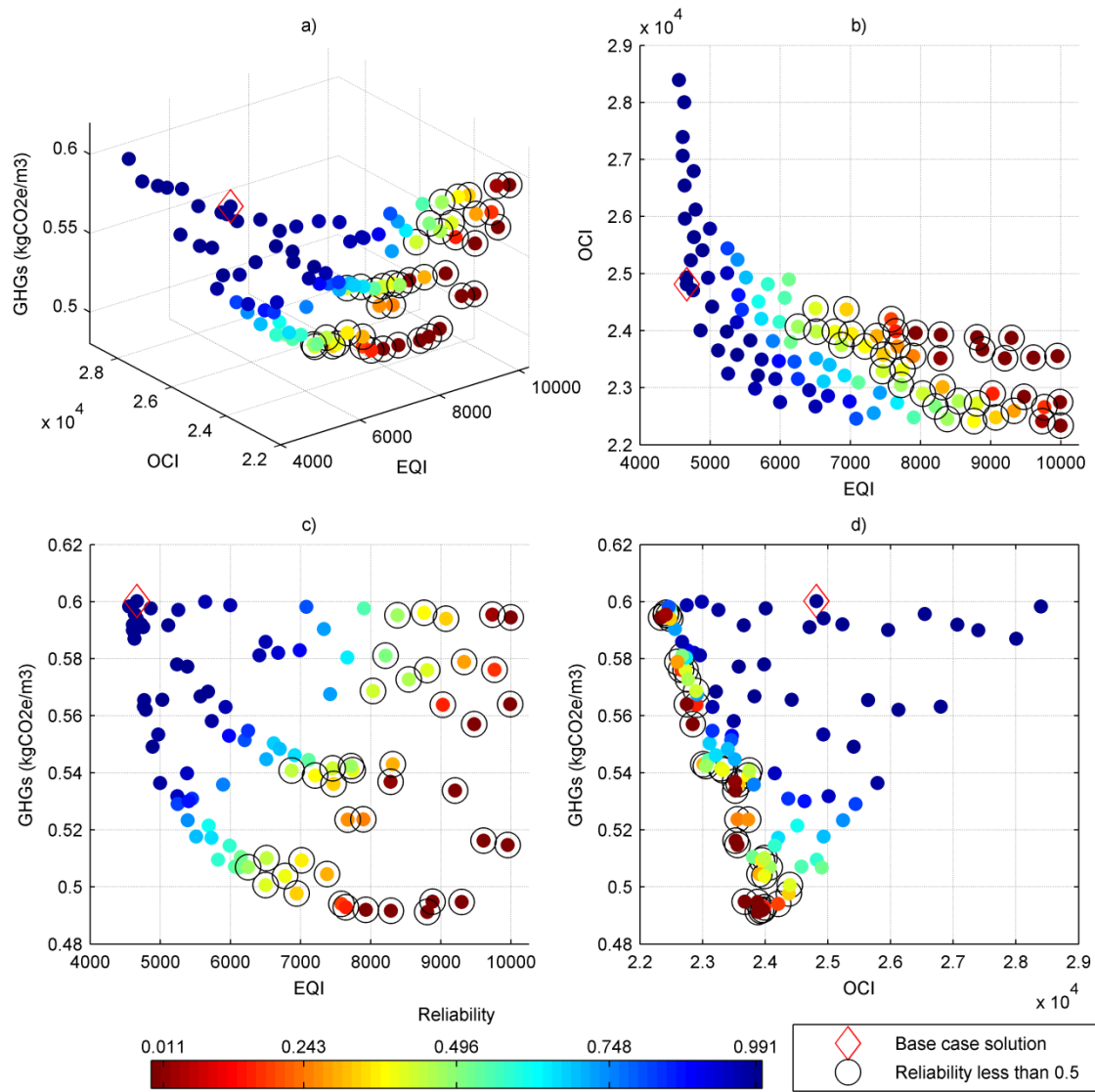


Figure A.11: Effluent total nitrogen reliability of non-dominated solutions bettering base case GHG emissions under default conditions, with solutions failing to a reliability of at least 0.5 identified

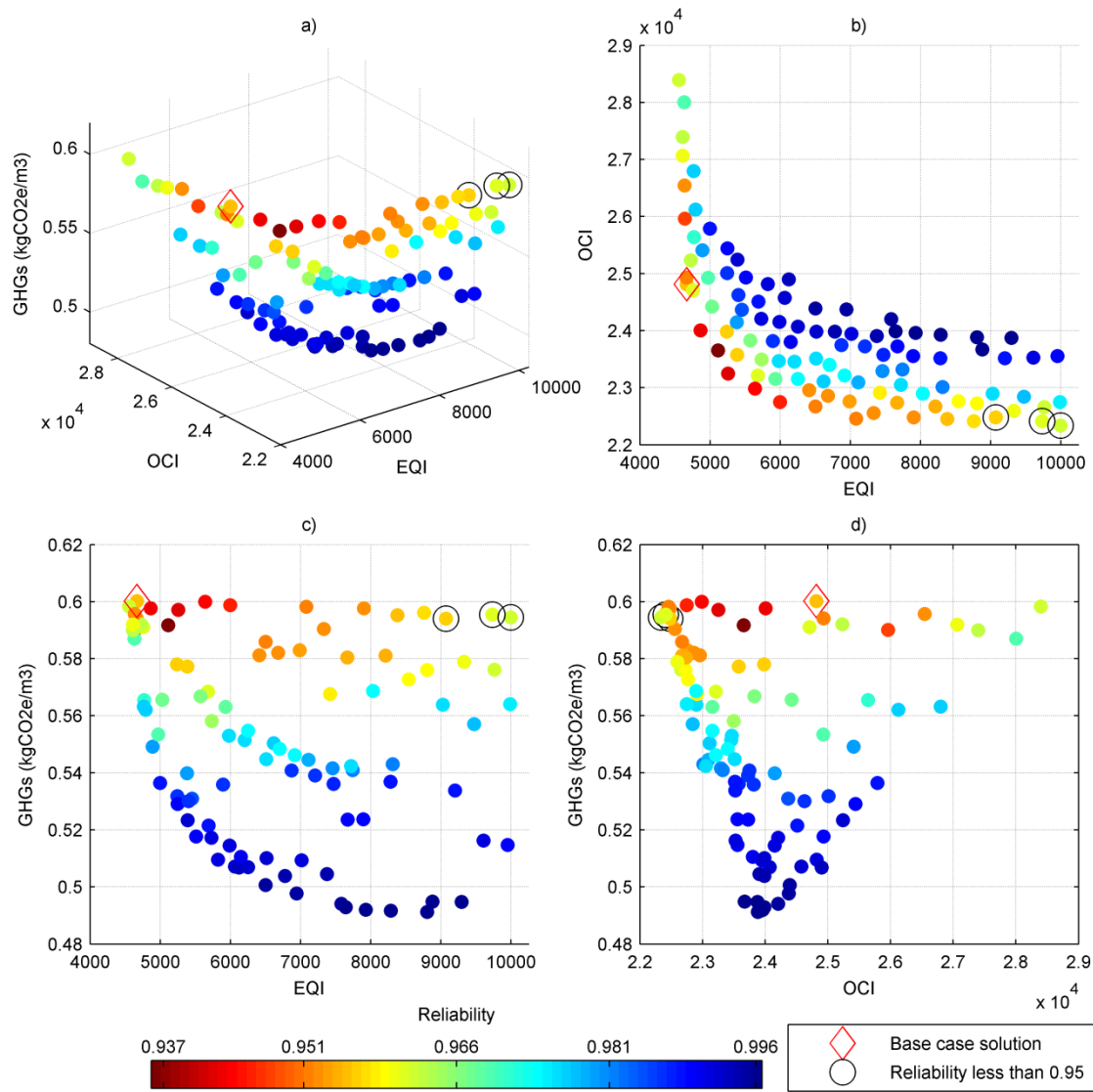


Figure A.12: Effluent GHG emission reliability of non-dominated solutions bettering base case GHG emissions under default conditions, with solutions failing to a reliability of at least 0.95 identified

Appendix E: Robustness Study – Complete Results

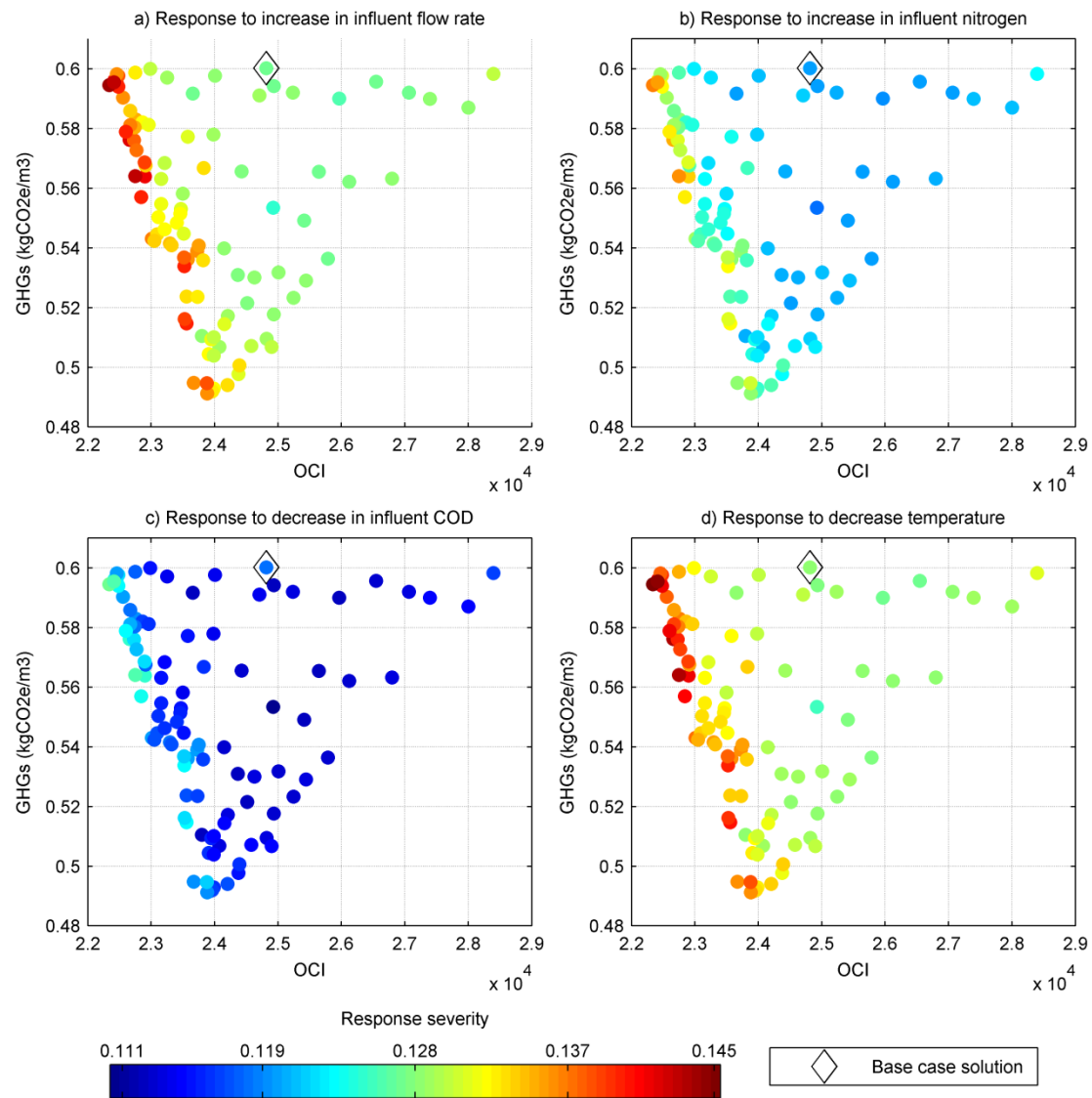


Figure A.13: Effluent BOD_5 response severities of non-dominated solutions bettering base case GHG emissions under default conditions

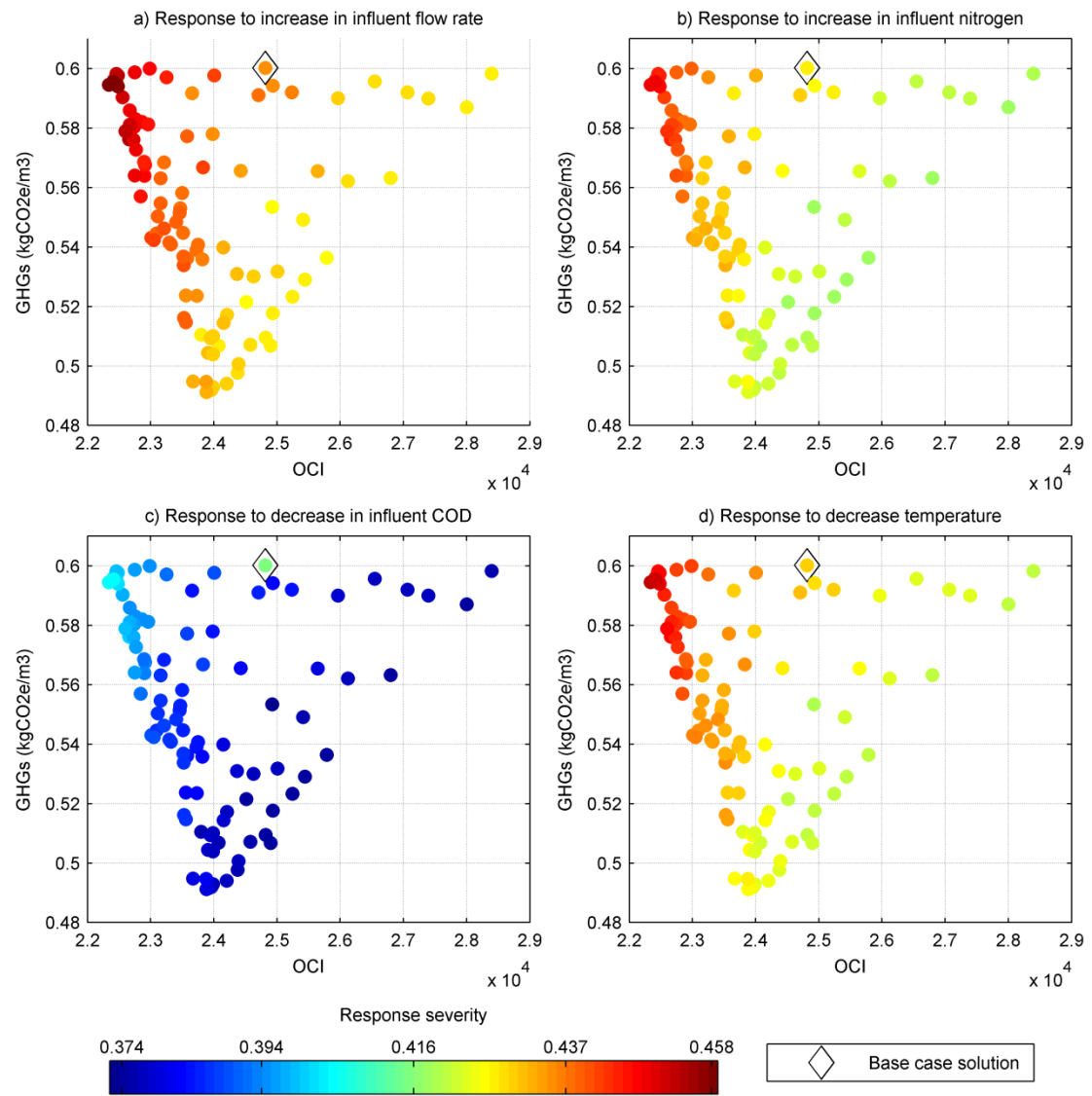


Figure A.14: Effluent COD response severities of non-dominated solutions bettering base case GHG emissions under default conditions

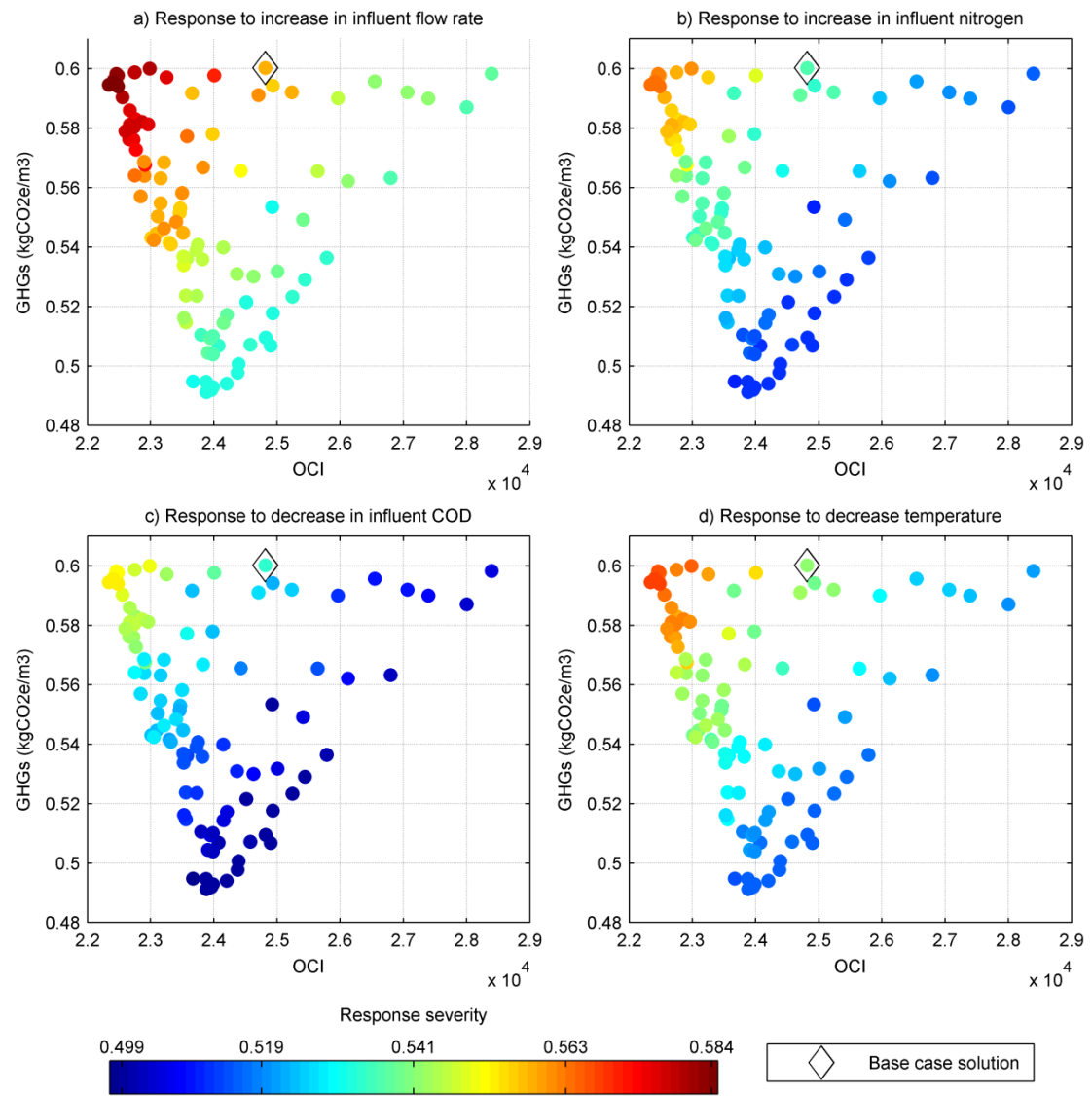


Figure A.15: Effluent TSS response severities of non-dominated solutions bettering base case GHG emissions under default conditions

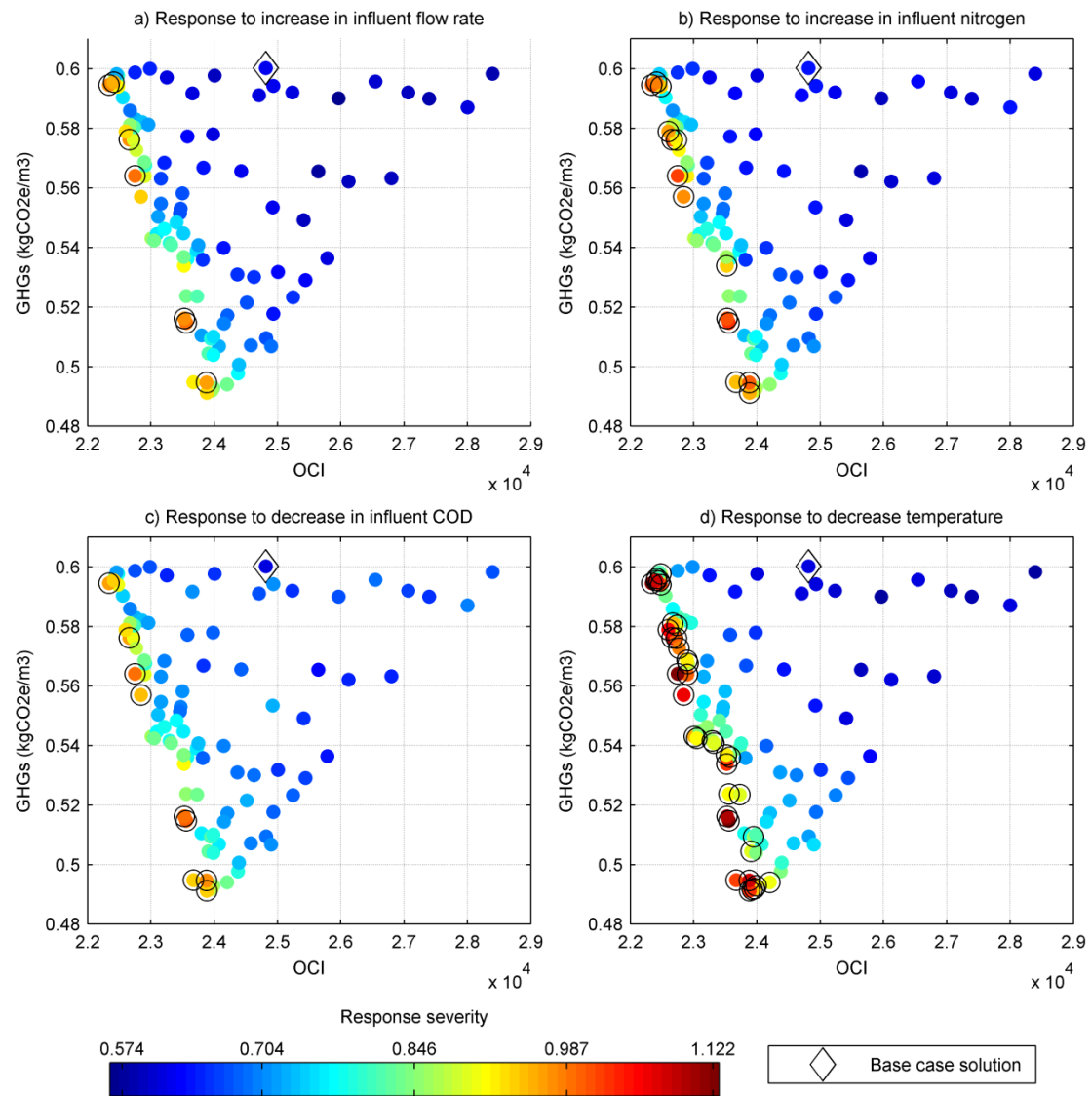


Figure A.16: Effluent total nitrogen response severities of non-dominated solutions bettering base case GHG emissions under default conditions, with solutions which reach failure point circled

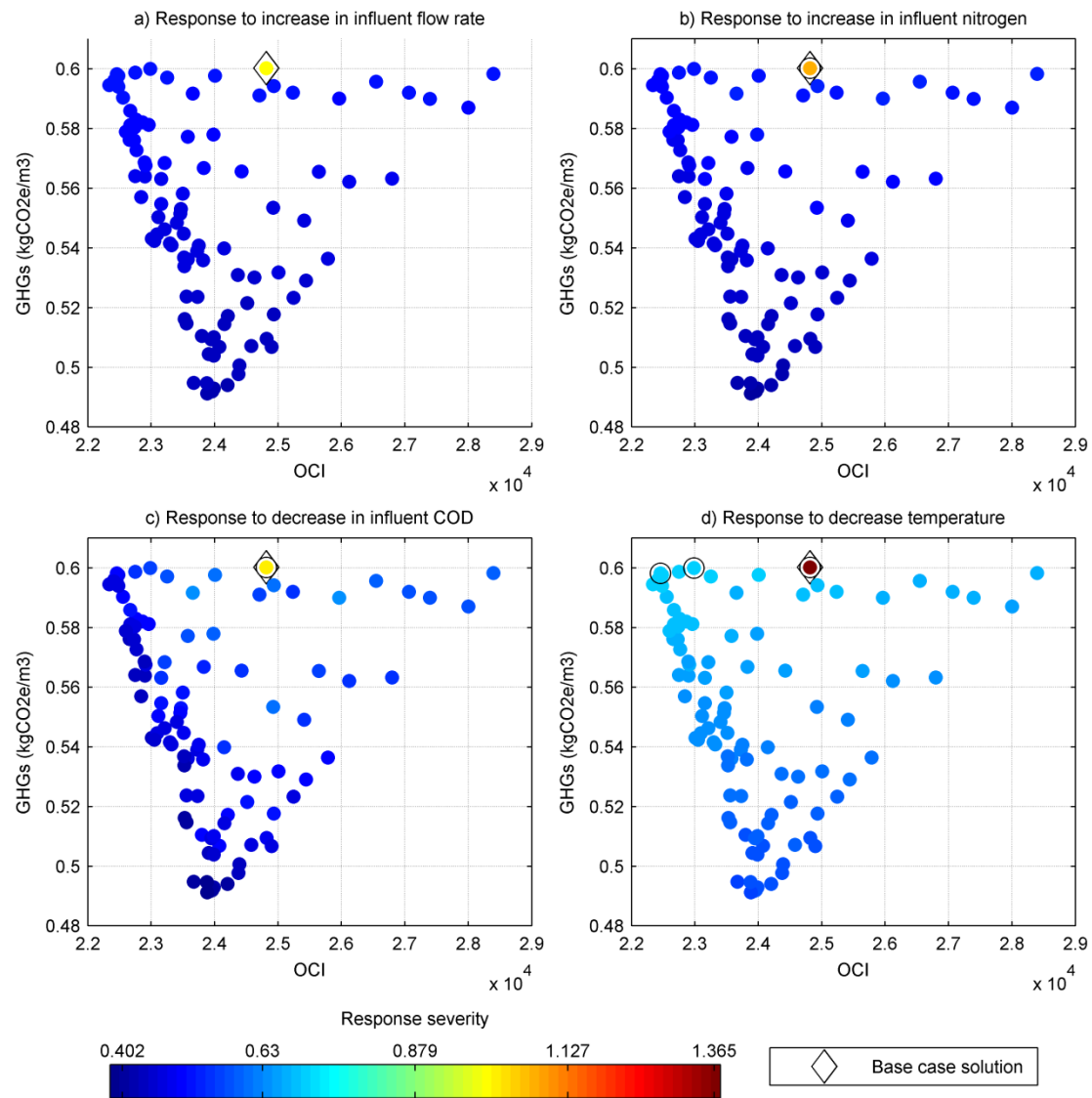


Figure A.17: GHG emission response severities of non-dominated solutions bettering base case GHG emissions under default conditions, with solutions which reach failure point circled

Appendix F: Resilience Study – Complete Results

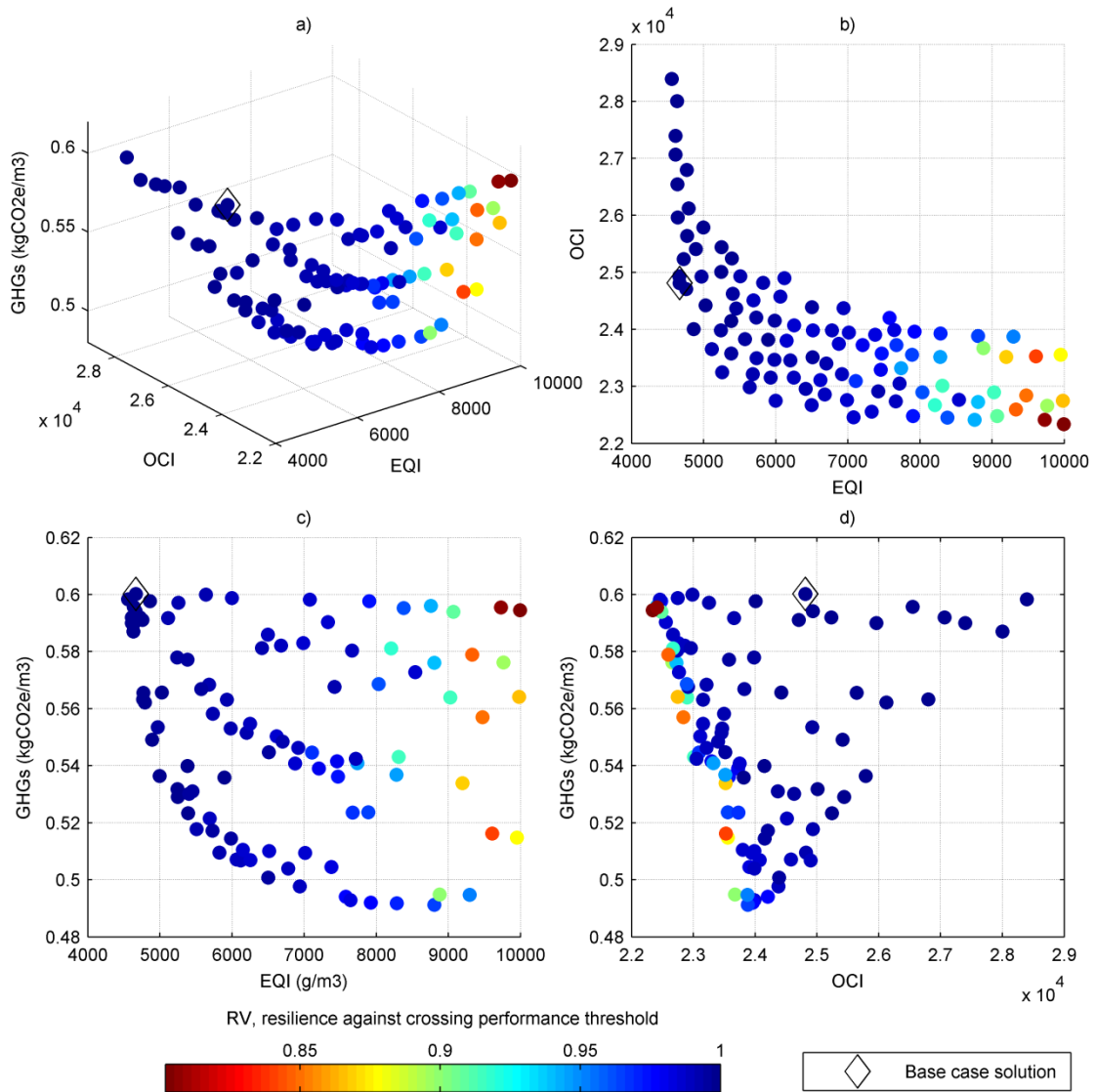


Figure A.18: Resilience against crossing a performance threshold (effluent total nitrogen) for non-dominated solutions bettering base case GHG emissions under default conditions

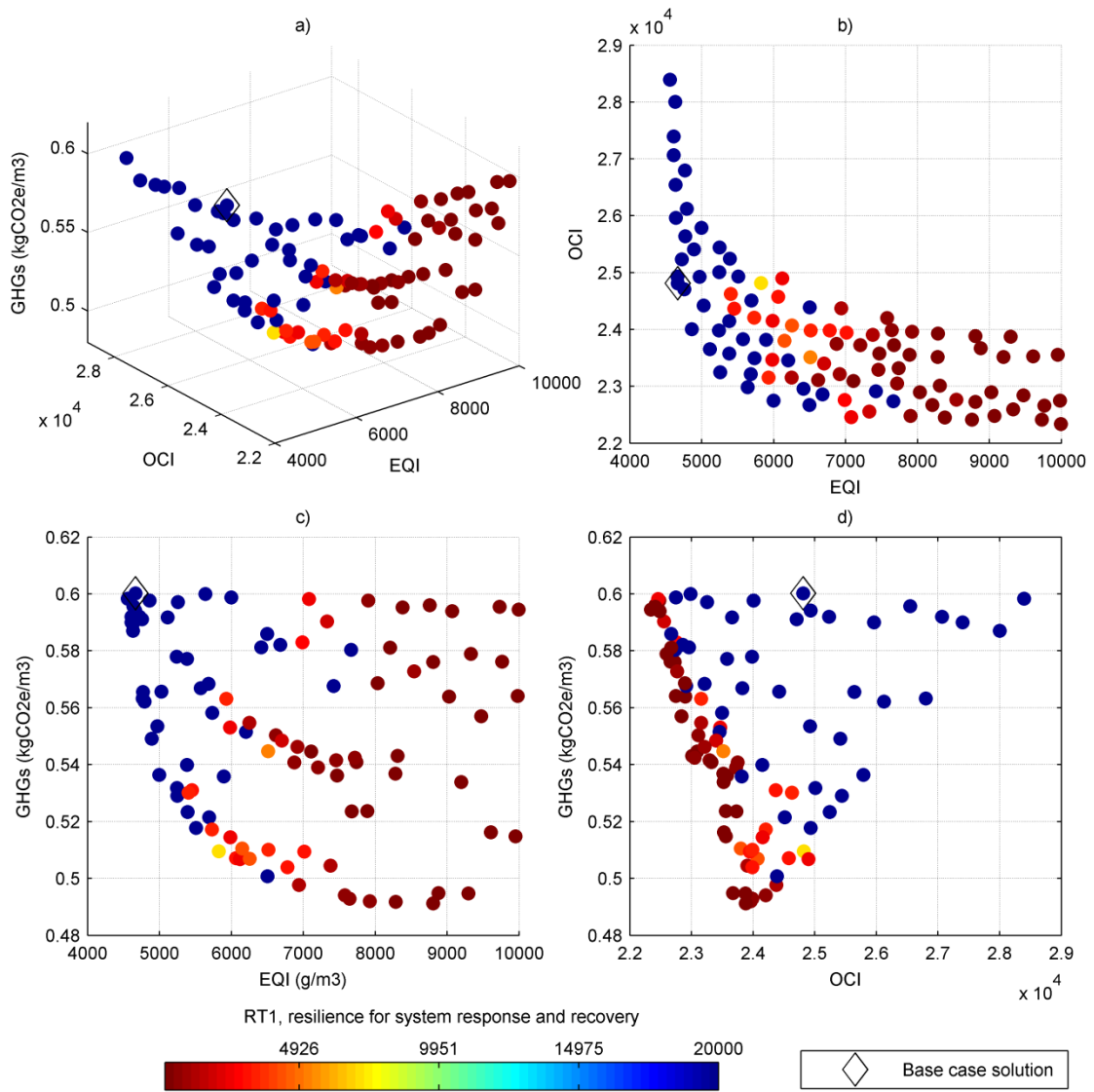


Figure A.19: Resilience for system response and recovery (R_{T1}) (effluent total nitrogen) for non-dominated solutions bettering base case GHG emissions under default conditions; solutions with $R_{T1} > 20000$ are shown as $R_{T1} = 20000$

Table A.1: Correlation coefficients for relationships between decision variable values and total nitrogen resilience indicators

Variable	R_V	R_{T1}	R_{T2}
Qintr (m ³ /d)	0.10	-0.09	-0.09
Qw (m ³ /d)	-0.08	-0.09	-0.09
KLa1 (/d)	0.03	-0.05	-0.05
KLa2 (/d)	-0.20	-0.15	-0.15
carb1 (m ³ /d)	0.07	0.11	0.10
carb2 (m ³ /d)	-0.12	-0.03	-0.03
carb5 (m ³ /d)	-0.08	-0.02	-0.02
Controller setpoint (g/m ³)	0.09	0.14	0.14
Controller offset	0.04	-0.08	-0.08
Controller amplification	0.10	-0.02	-0.02
Controller integral time constant	-0.16	-0.23	-0.23
KLa3 gain	-0.07	-0.07	-0.08
KLa5 gain	-0.12	-0.06	-0.06

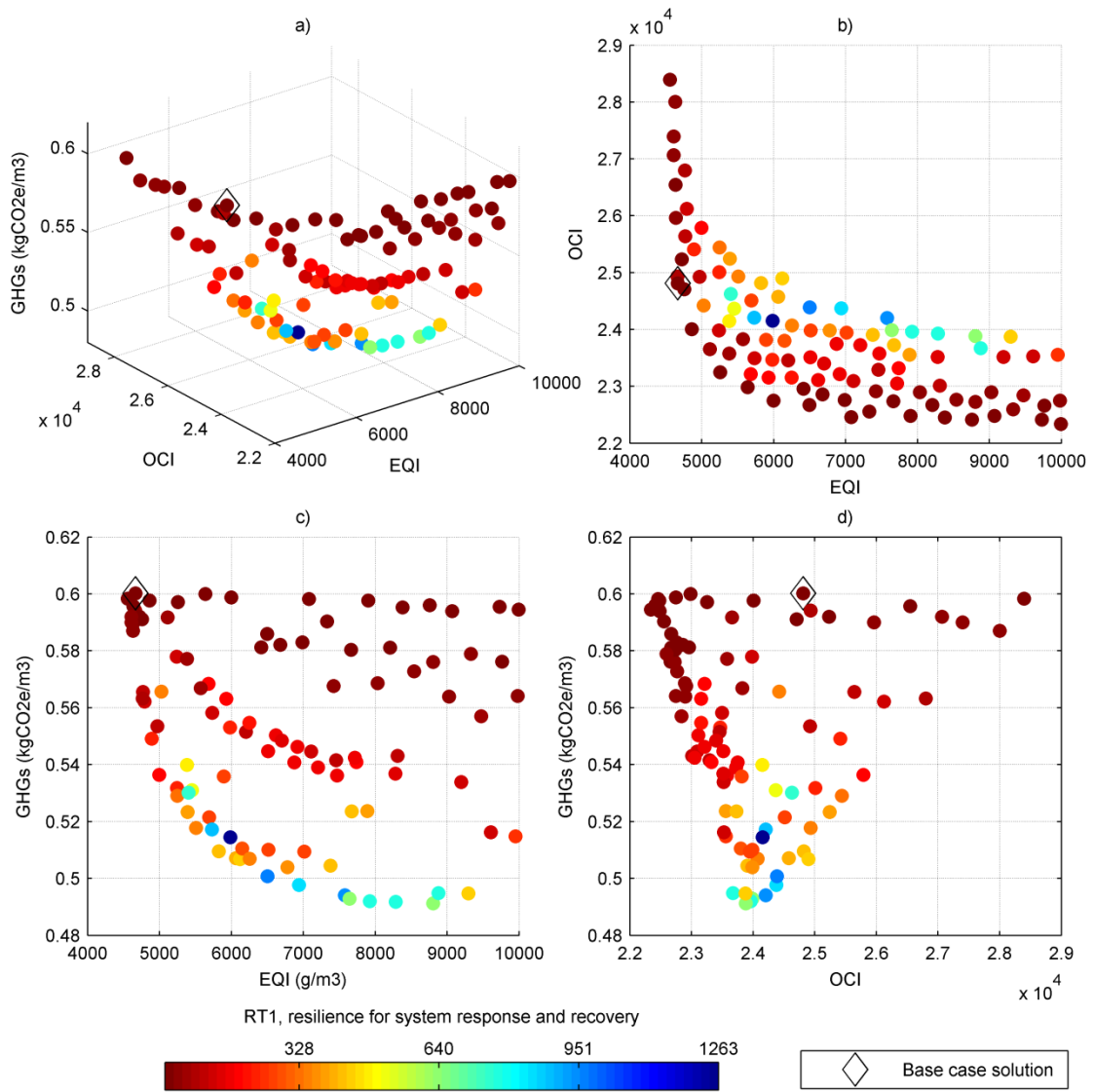


Figure A.20: Resilience for system response and recovery (R_{T1}) (GHG emissions) for non-dominated solutions bettering base case GHG emissions under default conditions

Table A.2: Correlation coefficients for relationships between decision variable values and GHG emission resilience indicators

Variable	R_V	R_{T1}	R_{T2}
Qintr (m ³ /d)	-0.22	0.03	0.04
Qw (m ³ /d)	0.34	0.28	0.34
KLa1 (/d)	-0.21	-0.09	-0.18
KLa2 (/d)	-0.02	0.06	-0.07
carb1 (m ³ /d)	0.20	0.05	0.23
carb2 (m ³ /d)	0.13	0.13	0.18
carb5 (m ³ /d)	0.05	-0.11	-0.07
Controller setpoint (g/m ³)	0.24	0.05	0.20
Controller offset	-0.02	0.22	0.24
Controller amplification	-0.08	0.00	-0.06
Controller integral time constant	-0.24	-0.20	-0.16
KLa3 gain	-0.21	-0.18	-0.06
KLa5 gain	-0.05	0.07	-0.03

Appendix G: Publications

1. Sweetapple, C. 2012. *Estimation of greenhouse gas emissions for development of adaptive wastewater treatment plant carbon management strategies: A literature review*, 13th IWA UK Young Water Professionals Conference, 18-20 April 2012, Exeter, UK
2. Sweetapple, C., Fu, G. & Butler, D. 2013. Identifying key sources of uncertainty in the modelling of greenhouse gas emissions from wastewater treatment. *Water Research*, 47(13), 4652-4665
3. Sweetapple, C., Fu, G. & Butler, D. 2014a. Identifying sensitive sources and key control handles for the reduction of greenhouse gas emissions from wastewater treatment. *Water Research*, 62, 249-259
4. Sweetapple, C., Fu, G. & Butler, D. 2014b. Multi-objective optimisation of wastewater treatment plant control to reduce greenhouse gas emissions. *Water Research*, 55, 52-62
5. Sweetapple, C., Fu, G. & Butler, D. 2014c. *Cost-efficient control of wastewater treatment plants to reduce greenhouse gas emissions*. IWA World Water Congress & Exhibition, 21-26 September 2014, Lisbon, Portugal

Estimation of greenhouse gas emissions for development of adaptive wastewater treatment plant carbon management strategies: A literature review

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Abstract This paper provides an in-depth analysis of the state-of-the-art methods and models for estimating greenhouse gas emissions from wastewater treatment plants (WWTPs), focusing on emissions arising due to biological processes and energy consumption. The methods and models identified are analysed with respect to their suitability for dynamic modelling of WWTPs for control strategy optimisation. Challenges are posed by the need to develop a model which incorporates existing methodologies for estimation of methane, carbon dioxide and nitrous oxide emissions and is suitable for dynamic modelling. Whilst existing models include methane and carbon dioxide process direct emissions, onsite energy consumption, biogas flaring or energy recovery, sludge disposal and embedded emissions from chemical use, the incorporation of nitrous oxide emissions would be beneficial. There is also scope to include more flexibility in terms of control strategies and to improve estimation methods where empirical formulae are still used.

Keywords Greenhouse gas emissions; Modelling; Optimisation

INTRODUCTION

The UK has committed to reducing its carbon emissions by 20% by 2020 and at least 80% by 2050 compared with 1990 levels. The water sector is estimated to be responsible for emitting 41 million tonnes of carbon dioxide equivalent (CO₂e) per year, of which up to 4.3 million tonnes can be attributed to wastewater pumping and collection, wastewater treatment and sludge to land processes (Defra, 2008). It is the fourth most energy intensive sector in the UK (Ainger et al., 2009) and, as such, it must contribute to the carbon reduction target, using a range of mitigation and adaptation strategies.

Increased water treatment as a result of the Water Framework Directive (WFD), however, has the potential to increase annual carbon dioxide emissions by more than 110,000 tonnes if there is no intervention, due to operational energy use and additional processes required (Georges et al., 2009). The water industry is therefore faced with the huge challenge of reducing carbon emissions by 80% whilst improving standards.

It is thought that significant emission reductions could be achieved by optimising existing processes in the urban wastewater system, with strategies including increasing operational efficiencies, redeveloping existing processes and promoting renewable energy generation. However whilst there has been significant research into the optimisation of wastewater treatment plant (WWTP) management strategies to increase efficiency, few attempts at optimisation have been made with the objective of minimising greenhouse gas (GHG) emissions. In order to develop a model that can be used to optimise carbon management control strategies, it is necessary to first identify appropriate GHG estimation methods. Many existing approaches are based on empirical formulae, using steady state calculations; however, whilst these can provide a useful indication of the likely emissions, they are unsuitable for use in optimisation as they do not allow for the effect of changing operating conditions and influent loads to be modelled. Models used must also allow the contribution of individual processes to direct and indirect GHG emissions to be determined.

This review therefore aims to analyse and assess existing methods and models with respect to their suitability for dynamic modelling of WWTPs for assessment of GHG emissions, and development of real time control strategies.

SCOPE OF WWTP EMISSION ESTIMATION MODELS

Following advances in GHG estimation techniques, a number of models have been developed for estimating GHG emissions from WWTPs and five of the most comprehensive are analysed in this paper. The main differences in the WWTPs modelled were due to the reactor design. All models used an anaerobic digester; none included aerobic digestion. The key features of the layouts modelled are as follows:

- Cakir and Stenstrom (2005) modelled both an anaerobic WWTP (with an anaerobic reactor and anaerobic digester) and an aerobic treatment plant (with an aerobic reactor and anaerobic digester) to enable a comparison of emissions from the two setups.
- Préndez and Lara-González (2008) utilised a range of existing models to estimate GHG emissions resulting from different components of the wastewater system, including both anaerobic and aerobic reactors.
- Shahabadi et al. (2010) considered a hybrid treatment system, with an anaerobic reactor followed by an anoxic/aerobic reactor.
- Flores-Alsina et al. (2011) adapted the IWA Benchmark Simulation Model No.2 (BSM2), and therefore used the same plant layout, which included an activated sludge reactor.
- Gori et al. (2011) used an activated sludge reactor.

The emissions accounted for in each of the aforementioned, recently published models are detailed in Table 1 to enable a comparison of different modelling approaches and the limitations of each. Emissions which were estimated using empirical relationships are identified, as they may produce results of questionable reliability if applied to systems with an unusual set up, and may not behave as predicted when control strategies are applied.

MODELLING OF DIRECT EMISSIONS

Direct emissions are classified as those which are emitted at the point of use and from a source that is either owned or controlled by the reporting entity. Wastewater treatment processes can result in the production of carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O), and further direct emissions may result from the combustion of fuels or fugitive emissions such as CH_4 leaks from pipes.

It can be seen from Table 1 that the choice of direct emission sources for inclusion in each model was similar. All included emissions from aerobic reactors, anaerobic digestion and, when part of the WWTP layout, anaerobic reactors. However emissions resulting from unintentionally anaerobic conditions and the stripping of CH_4 formed in the sewers were not considered and only one model included emissions from the biosolids dewatering unit.

Anoxic/aerobic reactors

Using aerobic wastewater treatment processes inhibits CH_4 production, although GHGs are not eliminated as CO_2 and N_2O are still produced. All WWTPs modelled incorporated aerobic reactors, but the extent to which their direct emissions were included varied; N_2O formation, for example, was only included only by Préndez and Lara-González (2008) and Flores-Alsina et al. (2011) due to the complexity of nitrogen conversion processes.

Table 1 Comparison of models used previously for estimation of GHG emissions from WWTPs

Source of emissions		Cakir and Stenstrom (2005)	Préndez and Lara-González (2008)	Shahabadi et al. (2010)	Flores-Alsina et al. (2011)	Gori et al. (2011)
Direct emissions	<u>Methane</u>					
	Stripping of dissolved methane formed in sewer system	×	×	×	×	×
	Poorly managed aerobic treatment	×	×	×	×	×
	Anaerobic reactor	✓T	✓E	✓T	×	×
	Anaerobic digester	✓T	✓T	✓T	✓T	✓T
	Biogas leakage	×	×	✓?	×	✓E
	Biosolids dewatering	×	×	×	×	✓E
	<u>Carbon dioxide</u>					
	Aerobic reactor	✓T	×	✓T	✓T	✓T
	Anaerobic reactor	✓E	✓?	✓T	×	×
	Aerobic digester	×	✓?	×	×	×
	Anaerobic digester	✓E	✓?	✓T	✓T	✓E
	Biogas leakage	×	×	✓?	×	✓E
	Biogas combustion	✓E	×	✓T	✓T	✓T
	<u>Nitrous oxide</u>					
	Nitrification and denitrification in wastewater treatment	×	✓E	×	✓T	×
	Nitrification and denitrification in sludge treatment	×	✓E	×	×	×
Indirect emissions	<u>Energy consumption</u>					
	Generic energy consumption / other equipment	×	✓E	✓E	×	✓E
	Pumping	×	×	×	✓E	✓E
	Aeration	✓E	×	✓E	✓?	✓E
	Heating	✓E	×	✓T	✓T	✓E
	Mixing	×	×	×	✓E	×
	<u>Embodied carbon</u>					
	Chemicals	×	×	✓E	✓E	×
	<u>Reactor effluent</u>					
	Stripping of dissolved methane	✓T	×	✓T	×	×
	Degradation of remaining biosolids	×	×	✓?	×	×
	Nitrification and denitrification	×	×	×	×	×
	<u>Digester effluent</u>					
	Transportation	×	×	✓E	✓E	×
	Stripping of dissolved methane	✓T	×	×	×	×
	Methane from degradation	×	✓E	✓T	×	×
	Carbon dioxide from degradation	×	✓E	✓T	✓E	×
	Nitrous oxide from nitrogen conversion	×	✓E	×	×	×

KEY: ✓E = Empirical method, ✓T = Method with theoretical basis,
 ✓? = Method not detailed, × = Not calculated

According to the IPCC (2006), CO₂ emissions from wastewater should not be considered in GHG inventories as they are of biogenic origin. As such, Préndez and Lara-González (2008) did not include CO₂ emissions from the aerobic reactor. However in order to develop a comprehensive model of GHG emissions resulting from wastewater treatment for the development of carbon management strategies, it is necessary to include all potential sources.

Cakir and Stenstrom (2005) related CO₂ emissions to BOD reduction only, utilising a yield factor 1.375 kg CO₂/kg BOD_u for the activated sludge process. The origin of this factor was not detailed, and it differs significantly from those used in other models and estimation methodologies. Shahabadi et al. (2010) and Flores-Alsina et al. (2011) provided a more detailed methodology, attributing CO₂ emissions to a number of different processes occurring within the reactor and using stoichiometry to derive theoretical emission factors. However each used different formulae to represent utilisation of carbonaceous BOD and biomass decay, therefore resulting in significantly different emission factors: 0.33 g CO₂/g COD and 1.56 g CO₂/g VSS for Shahabadi et al. (2010) and 1.1 g CO₂/g O₂ (equivalent to 1.1 g CO₂/g COD) and 1.95 g CO₂/g VSS for Flores-Alsina et al. (2011).

Shahabadi et al. (2010) also included CO₂ emissions resulting from nutrient removal activities to improve the completeness of the model. They assumed that nitrogen removal is carried out by the nitrification-denitrification process and used stoichiometric relationships to derive emission factors of 2.62 g CO₂/g N-nitrate and 2.81 g CO₂/g N-nitrate for denitrification with and without an external carbon source respectively.

The model developed by Flores-Alsina et al. (2011) made allowance for CO₂ utilisation during nitrification, applying this as CO₂ credit. CO₂ credit was calculated using an emission factor of 0.31 g CO₂/g N nitrified.

Nutrient removal activities can also result in emissions of N₂O from the reactors. Préndez and Lara-González (2008) included GHG emissions from incomplete nitrification and denitrification in their model, but the method was based upon the use of activity data (e.g. population served) and empirical emission factors, and would therefore be unsuitable for use in control strategy optimisation. Flores-Alsina et al. (2011) included N₂O emissions from heterotrophic denitrification in the water line, as calculated by the modified Activated Sludge Model for Nitrogen (ASMN), but did not consider emissions due to incomplete nitrification.

Anaerobic reactor

When treatment is carried out under anaerobic conditions, the biogas produced contains both CO₂ and CH₄ and has a significant global warming potential (GWP). Emissions from anaerobic reactors, where modelled, were typically estimated using emission factors. Préndez and Lara-González (2008) again utilised activity data and empirical emission factors and their model might, therefore, produce results of questionable reliability if used in the development of control strategies.

The model of Cakir and Stenstrom (2005) offered some improvement, in that they utilised the modelled reaction kinetics and made allowance for some of the CH₄ produced entering solution in accordance with Henry's Law. However they only considered CH₄ and CO₂ production associated with BOD reduction using emission factors of 0.25 g CH₄/g BOD_u and 0.69 g CO₂/g BOD_u, respectively, for which no explanation was given. The CO₂ emission factor differs significantly from that given by Shahabadi et al. (2010) of 0.27 g CO₂/g BOD, which was derived from stoichiometry, and might therefore provide an overestimate. The CH₄ emission factor used in both models is of questionable reliability, as the stoichiometric relationship provided yields a factor of 0.25 g CH₄/g COD (not BOD).

Shahabadi et al. (2010) offered further improvement by including biomass decay as a contributing factor to emissions from the anaerobic reactor. Emission factors of 0.35 g CH₄/g VSS and 0.58 g CO₂/g VSS were used, based on the theoretical reaction equation provided.

Anaerobic digester

Production of CO₂ and CH₄ in the anaerobic digester was included in all of the models compared, using a range of different methods. As for the anaerobic reactor, Cakir and Stenstrom (2005) included only emissions resulting from BOD oxidation, using the theoretical CH₄ yield factor for COD reduction to estimate emissions due to BOD reduction. Allowance was made for CH₄ dissolved in the digester effluent (calculated using Henry's Law) when estimating the biogas composition.

Shahabadi et al. (2010) stated that their method for estimating emissions from the anaerobic digester was similar to that for the anaerobic reactor, which included calculation of GHG production during BOD reduction and biomass decay using theoretical emission factors; however the differences were not explained beyond the fact that it was assumed 70% of the available biomass in the digester degraded.

The existing Anaerobic Digestion Model No.1 (ADM1, as incorporated in BSM2) was used by Flores-Alsina et al. (2011) to calculate both CH₄ and CO₂ emissions from anaerobic digestion.

Gori et al. (2011) calculated CH₄ production in the anaerobic digester due to COD oxidation only, using a theoretical emission factor of 0.35 Nm³ CH₄/kg bCOD, derived from stoichiometry. CO₂ production was estimated empirically, based on the calculated CH₄ production and an assumption that this constitutes a fixed proportion of the biogas; this method makes no allowance for changing biogas composition resulting from different operational parameters.

Préndez and Lara-González (2008) also modelled N₂O emissions resulting from incomplete nitrification and denitrification during sludge treatment. However, as for the reactor, the calculation used activity data and empirical emission factors and would therefore be unsuitable for providing an accurate indication of the effects of adjusting operational procedures.

Biogas leakage and combustion

Biogas has a high potential energy and is commonly combusted for heating or electricity generation. This results in the conversion of CH₄ and oxygen to CO₂ and water, which is preferable due to the lower GWP of the emissions (Monteith et al., 2005).

CO₂ emissions from the combustion of biogas were generally included in models, although the technique was not always clear. The method provided by Cakir and Stenstrom (2005), for example, was particularly ambiguous, being based upon the anaerobic reactor and digester oxygen requirement and a CO₂ yield factor in terms of kg CO₂/kg BOD_u. The remaining models used a theoretical emission factor of 2.75 g CO₂/g CH₄, based on stoichiometry, in conjunction with the modelled CH₄ production. This relies on the assumption that all CH₄ is fully combusted. If combustion is incomplete, however, then this will impact on both direct and indirect emissions: direct emissions will have a higher GWP than calculated due to the presence of non-combusted CH₄ and indirect emissions resulting from energy generation will be higher due to a lower offset from energy recovery than calculated.

Some biogas could also be leaked directly to the atmosphere, therefore reducing energy recovery and increasing the GWP of emissions as some CH₄ does not undergo combustion. Allowance for biogas leakage was made by Shahabadi et al. (2010) and Gori et al. (2011), although the latter only

included CH₄ emissions, which were assumed to be 2% of the biogas generated. The method used by Shahabadi et al. (2010) for quantifying leaks was not provided.

Biosolids dewatering

Emissions released during biosolids dewatering were modelled only by Gori et al. (2011) and the method used was not explained in detail. It was assumed that half of the CH₄ contained in the biogas-saturated biosolids was released directly to the atmosphere during dewatering and the rest recirculated and converted to CO₂ during biological oxidation; however it is unclear how the CH₄ content of the biosolids was determined.

MODELLING OF INDIRECT EMISSIONS

Emissions from a source not owned or controlled by the reporting entity but which occur as a result of their activities are classified as indirect emissions. In the context of a WWTP, these include emissions associated with the generation of electricity for onsite use, processing of chemicals and waste disposal. The inclusion of indirect emissions in models was generally less complete than direct emissions. Préndez and Lara-González (2008), for example, only included calculation of emissions from the degradation of digester effluent and generic energy consumption.

Energy consumption

Indirect emissions resulting from energy consumption were modelled in all five of the models compared, based on the generation of power imported and/or the combustion of biogas as a renewable energy source. Calculation of emissions attributed to power generation varied greatly: Cakir and Stenstrom (2005) and Gori et al. (2011), for example, used emission factors of 0.96 kg CO₂e/kWh and 0.245 kg CO₂e/kWh respectively and neither provided any justification for the values chosen. This large variation is not unexpected, as previous studies have used factors within the range 0.21 – 0.77 kg CO₂e/kWh to account for differences in the energy generation mix (Sahely et al., 2006); however it means that the choice of emission factor could have a significant effect on the calculated overall GHG emissions.

A range of methods were used to estimate the energy requirement of the WWTP, although they were generally more comprehensive in later models. Typically only the most energy intensive operations (including pumping, aeration, heating and mixing) were considered (Cakir and Stenstrom, 2005; Shahabadi et al., 2010; Flores-Alsina et al., 2011).

When calculating the energy required for aeration, several models utilised empirical formulae to provide a basic estimate, however the emission factors varied considerably. Cakir and Stenstrom (2005), for example, used a fixed aeration efficiency of 2 kg O₂/kWh, whereas Shahabadi et al. (2010) used a factor of 7.2 g O₂/kJ (equivalent to 25.9 kg O₂/kWh). This large variation suggests that such a method of calculation may not be robust. Furthermore, Shahabadi et al. (2010) calculated aeration energy based on the oxygen demand of the aerobic reactor, therefore making the assumption that the oxygen supplied is equal to the oxygen required. Whilst this method could be used in carbon accounting and control strategy development to provide an indication of likely energy use, accuracy could be improved by taking into account the effect of aeration rate on efficiency. Flores-Alsina et al. (2011) used the aeration energy calculation within the BSM2, which is based upon a more detailed methodology, valid specifically for Degremont DP230 porous disks at an immersion depth of 4m.

Flores-Alsina et al. (2011) also modelled the energy required for mixing and pumping using the original BSM2, in which pumping energy is related linearly to the volume of water pumped, using different emission factors for each pumping location. Similarly, Gori et al. (2011) used a fixed

specific energy consumption (kWh/m^3) for influent pumping. This method makes no allowance for the maximum pumping capacity and the effect of flow rate on efficiency.

When modelling the energy required for heating of the anaerobic digester, Gori et al. (2011) related it only to the mass of sludge treated, using an empirical emission factor of $0.16 \text{ kWh/kg dry solids}$. This implies that power used is linearly related to the mass of sludge treated, which may not be a valid assumption during dynamic modelling if there is temporal variation in influent temperature. Shahabadi et al. (2010) provided a more versatile method for calculating the energy required for heating, based on a specific heat of $4,200 \text{ kJ/kg/}^\circ\text{C}$ for wastewater, the modelled influent temperature and flow rate and the required digester temperature.

Models typically offset the energy requirement of the plant with the energy recovery from CH_4 combustion. Methods used to calculate energy recovery from biogas were similar and typically applied a heat conversion efficiency of 0.83 (Cakir and Stenstrom, 2005; Shahabadi et al., 2010) or an electricity generation efficiency of 0.43 (Flores-Alsina et al., 2011) to the theoretical energy content of the CH_4 combusted (50 MJ/kg CH_4). Gori et al. (2011) used the same method, but with a specific energy of $35.8 \text{ MJ/m}^3 \text{ CH}_4$ and an energy recovery efficiency of 0.5. This method provides a straightforward means of estimating energy generation; however given that the density of CH_4 varies with temperature it would be preferable to specify the specific energy of CH_4 in terms of mass, not volume. Furthermore, allowance should be made for instances when the energy demand is less than the energy recovered. Unless the surplus energy is stored in these cases, the average energy offset across the simulation period would be less than the energy recovery calculated based on only the conversion efficiency and theoretical energy content.

Embodied carbon

Indirect emissions due to the use of chemicals during treatment were included in only two of the models compared. Shahabadi et al. (2010) used emission factors of $1.74 \text{ g CO}_2/\text{g}$ and $1.54 \text{ g CO}_2/\text{g}$ for the production and transmission of alkalinity and methanol respectively, having calculated the mass of chemicals used during treatment processes from stoichiometric equations. Flores-Alsina et al. (2011) only considered external carbon source (methanol) addition, for which the same emission factor was used. Whilst these emission factors were both derived empirically, they could be used in dynamic modelling and assessment of control strategies provided that the mass of chemicals used was calculated accurately, as emissions resulting from chemical production should be unaffected by changes in their end use. Embodied carbon should not be overlooked in the development of a comprehensive model, as a previous study (Shahabadi et al., 2009) found that over 50% of total GHG emissions from an anaerobic treatment plant could be attributed to material usage.

Reactor effluent

Stripping of dissolved CH_4 from the reactor effluent was not commonly included in the models, however where it was assumed that all CH_4 produced was emitted at source (with none entering solution) it would be inappropriate to do so. Cakir and Stenstrom (2005) and Shahabadi et al. (2010) used Henry's Law and the partial pressure of CH_4 in the anaerobic reactor gas to estimate the mass of CH_4 dissolved in the effluent, and then assumed that all dissolved CH_4 would be later stripped to the atmosphere. Modelling the processes of CH_4 being dissolved in the reactor and subsequently stripped from the effluent has no effect on net emissions from the WWTP (as it is assumed that all CH_4 generated is released at some stage, provided that biogas from the reactor is not combusted) and is therefore not essential when calculating total emissions; however it would be of significance if a distinction between direct and indirect emissions is required.

Digester effluent

Stripping of dissolved CH₄ from the digester effluent was included in two models: Cakir and Stenstrom (2005) and Shahabadi et al. (2010) estimated the mass of CH₄ dissolved in the sludge using Henry's Law, as for the anaerobic reactor effluent. The BSM2, as used by Flores-Alsina et al. (2011), includes calculation of the CH₄ in solution in the digester; however stripping of CH₄ remaining in the effluent was not modelled. Given that biogas from the digester is usually combusted, making allowance for CH₄ dissolved in the effluent could result in an increase in the CO₂e of emissions, as it would not be converted to CO₂ (which has a lower GWP). Furthermore it would reduce the energy recovery from biogas combustion, therefore reducing the energy offset and increasing indirect emissions due to the generation of imported energy.

Transportation of sludge can result in further indirect emissions, although these have been included in few models. Flores-Alsina et al. (2011) used an unspecified emission factor (kg CO₂e/mile/tonne sludge). An emission factor of this form could reasonably be used during dynamic modelling of systems as, within the context of developing WWTP control strategies, no changes could be made which would affect the transport efficiency.

Indirect emissions from the degradation of digester effluent have been included, to varying extents, in emission estimation models. Shahabadi et al. (2010), for example, assumed that biomass in the digester effluent degrades anaerobically downstream, although did not specify whether this was modelled in accordance with the stoichiometric relationship used previously to represent biodegradation of biomass in the anaerobic digester or by other means. N₂O emissions from the degradation of sludge were generally omitted; Préndez and Lara-González (2008) identified sludge disposal to landfill or agricultural use as a source of N₂O emissions, but their referenced methodology for calculating emissions only included N₂O from sludge incineration. Where included, indirect N₂O emission models were based on empirical formulae; this could be attributed to the complexity of nitrogen conversion processes and lack of simple models. Whilst models with a theoretical basis would be preferable for the modelling of dynamic systems and assessment of control strategies, an empirical formula relating indirect N₂O emissions to the nitrogen content of the effluent could be used as offsite processes would be independent of the WWTP operational procedure.

MODEL CALIBRATION AND VERIFICATION

GHG emission estimates from the five models analysed were uncalibrated, despite some models being applied to real WWTPs and using measured process parameters. Préndez and Lara-González (2008) incorporated a range of existing models, modified to fit the national conditions and specific scenarios, but did not test the validity of these modifications with real data. This could be attributed partly to a lack of data and difficulties in obtaining a comprehensive set of measurements – particularly for indirect emissions.

Some attempts were made to validate calculated emissions using previously published values. For example, the relationship between the gas phase percentages of biogas constituents and influent substrate concentration modelled by Cakir and Stenstrom (2005) were plotted and compared with a plot of compositions reported in literature. However whilst similar trends were observed, the magnitude varied considerably; for instance an influent substrate concentration of 10,000 mg COD/L yielded a modelled gas with 54% CH₄ and 42% CO₂, whereas previously published studies reported compositions in the region of 76% CH₄ and 19% CO₂. As such, there could be significant error in the modelled CH₄ production and subsequent energy recovery.

Emission estimates modelled by Shahabadi et al. (2010) were compared with those obtained in two previous studies, using the same process parameters, in order to obtain an indication of their validity. It was found that the emissions per unit volume of wastewater treated were similar to those reported by Monteith et al. (2005), who used data from an activated sludge plant for calibration. However the calibration data was very limited in terms of GHG production, containing only the total volume of gas produced in the anaerobic digester and no details of its CH₄ and CO₂ content. Additionally when emissions modelled by Shahabadi et al. (2010) were expressed per unit mass of COD removed, results differed considerably from those reported in literature – this was attributed to differences in wastewater composition and the inclusion of offsite GHG emissions.

Flores-Alsina et al. (2011) made no attempt at calibration, with the justification that the purpose of their model was to provide a means of including GHG emissions when assessing overall WWTP performance rather than predicting emissions with complete accuracy. It was argued that the range of estimates obtained when modelling different scenarios were within the range of values presented in two previous publications, however the variation in these values was large (0.34 – 2.2 kg CO₂e/m³) and individual results for specific scenarios were not compared.

MODEL OMISSIONS

From Table 1 it can be seen that some sources of emissions were omitted from all models. Unaccounted for emissions of CH₄ and N₂O in particular could have a significant impact on the overall GWP. Emissions due to the stripping of CH₄ formed in the sewer system, for example, were not included in the comprehensive emission estimation models but experimental evidence (Guisasola et al., 2008) has shown that CH₄ formation in the sewer system could increase CH₄ emissions from WWTPs by 12 - 100 %. However there is currently a high degree of uncertainty when estimating these emissions. Guisasola et al. (2009) found that there is a high correlation between CH₄ production and hydraulic residence time (HRT) and the pipe area to volume ratio (A/V), with higher CH₄ concentrations corresponding to a long HRT or large A/V ratio; but whilst it was concluded that CH₄ production in sewers may provide a significant contribution to overall GHG emissions from the wastewater system, dissolved CH₄ stripped within the WWTP boundary was not quantified.

Similarly, direct CH₄ emissions from resulting from poorly managed treatment and unintentionally anaerobic conditions were not modelled due to a lack of reliable estimation techniques; however they could be significant, as a recent full-scale investigation (Wang et al., 2011) recorded CH₄ emissions at every processing unit in the WWTP. The omission of CH₄ emissions from poorly managed aerobic treatment could affect the validity of results when attempting to optimise control strategies; for example existing emission estimation methods for aerobic processes may suggest that reducing aeration would lower overall emissions due to a reduction in electricity consumption, however in reality conditions may become anaerobic, therefore resulting in the production of CH₄ and greatly increasing the GWP of emissions.

Calculation of indirect emissions of N₂O was very limited, with no models including formation of N₂O from the reactor effluent. This could be a significant omission, as several authors (IPCC, 2006; Préndez and Lara-González, 2008; Kampschreur et al., 2009) have highlighted the importance of N₂O emissions from receiving waters, most commonly attributed to further nitrification and denitrification. Kampschreur et al. (2009) added that stripping of dissolved N₂O formed during treatment is slow due to its relatively high solubility in water and may be completed outside the boundary of the WWTP, therefore contributing to offsite N₂O emissions. This theory is, however, contradicted by Foley et al. (2010), who recorded less than 5 % of N₂O formed in the WWTP

dissolved in the effluent and argued that N_2O is quickly stripped to the atmosphere due to its high mass transfer coefficient.

MODEL APPLICATIONS

The models detailed above were used to assess the GHG emissions resulting from wastewater treatment under a number of scenarios, including different treatment types (Cakir and Stenstrom, 2005; Préndez and Lara-González, 2008), variations in influent characteristics (Cakir and Stenstrom, 2005; Shahabadi et al., 2010; Gori et al., 2011) and different control strategies (Flores-Alsina et al., 2011).

Préndez and Lara-González (2008) modelled GHG emissions resulting from six scenarios (incorporating varying proportions of biogas reuse and aerobic and anaerobic treatment). During the period in which 100% of wastewater was treated in a WWTP, it was found that the treatment processes and management strategies yielding the lowest emissions (per m^3 of water treated) consisted of 90% aerobic and 10% anaerobic wastewater treatment, 100% anaerobic sludge treatment and 75% biogas reuse. This approach is only meaningful when designing new WWTPs or carrying out extensive modifications to the plant design; if embodied carbon were included in the emission estimation then it is likely that any major structural changes would not be a feasible solution. Furthermore the investigation had a very limited scope, with only six discrete scenarios modelled and a maximum of 75% biogas reuse considered. However given that the majority of emission sources were modelled using activity data and empirical emission factors, it would not be feasible to use this model for a detailed analysis as results would be of insufficient accuracy.

In order to identify the most efficient treatment process (in terms of GHG production), Cakir and Stenstrom (2005) modelled the effect of influent BOD_u on net CO_2e production for anaerobic and aerobic systems with a range of solids retention times (SRTs). From this it was concluded that aerobic treatment results in lower emissions when the influent BOD_u is low, with anaerobic treatment becoming increasingly competitive as influent BOD_u increases and yielding negative net emissions when the influent BOD_u is greater than 800 mg/L. However no assessment of the treatment efficiency or effluent quality was made and ensuring compliance with legislative standards could affect the calculated emissions. Application and optimisation of control strategies could also have a significant impact on the reported relationship between influent BOD_u and net CO_2e production. Furthermore, the results are of questionable reliability as the model was not calibrated and significant differences between the modelled digester gas composition and compositions previously reported in literature were identified.

Shahabadi et al. (2010) also carried out simulations with a range influent concentrations, both with and without energy recovery from biogas, but undertook a more detailed analysis of the effect of the influent characteristics on emissions from each process. The manufacture and transportation of alkalinity and methanol, for example, was identified as major source of GHG generation, suggesting that reduction of their use through efficient process control and optimisation has the potential to reduce overall emissions associated with wastewater treatment. Based on a comparison of the relative contribution of each source to overall emissions, a number of strategies to reduce emissions were recommended. However many of these recommendations, such as “increased energy efficiency to reduce electricity needs” and “increased efficiency of the anaerobic digester to produce more biogas” were vague, with no guidance on how they might be achieved. Additionally the effects of following more specific recommendations, such as operating the anaerobic digester at a lower temperature to reduce energy used for heating, were not modelled to investigate the associated trade-offs and confirm that they had the desired effects.

Gori et al. (2011) gave a more thorough investigation into the effects of soluble and particulate substrate concentrations on the carbon footprint of wastewater treatment processes: a range of pCOD/VSS influent ratios were tested and sensitivity analysis was carried out to determine the relative parameter variation within the range of influent concentrations modelled. It was found that increasing pCOD/VSS had the greatest impact on CO₂e resulting from biogas combustion and leakage, and caused a reduction in CO₂e from activated sludge respiration and biosolids dewatering.

The only testing of WWTP control strategies with respect to GHG emissions was carried out by Flores-Alsina et al. (2011). Three closed loop control strategies (relating to the dissolved oxygen (DO) set point, aeration flow and internal recycle flow rate) were simulated and compared with an open loop base case scenario. It was found that control strategies could be implemented to simultaneously reduce GHG emissions by up to 9.6%, reduce operational costs and improve effluent quality. This included a substantial reduction in aeration energy due to the implementation of a DO controller to improve efficiency of the aeration system and prevent nitrite accumulation. A detailed analysis of the relationship between DO set point, SRT and reactor COD/N ratio and the emissions from each processing unit modelled was also carried out. One of the findings from this analysis was that decreasing the SRT results in a reduction in net emissions due to increased CO₂ credit from energy recovery. This supports the modelled results of Cakir and Stenstrom (2005), in which the total CO₂ production from the WWTP more than doubled when the SRT was increased from 10 days to 30 days.

FUTURE CHALLENGES

Several of the models analysed were used to assess the impacts of changing influent conditions on GHG emissions. However given that the influent characteristics are (largely) beyond the control of the water companies, this information would be of minor importance when developing strategies to meet the CRC requirements whilst ensuring compliance with the WFD. It would be desirable to also consider the effects of adjusting the WWTP operational or control strategies. This would enable different approaches to be evaluated with respect to a number of criteria, including overall emissions, effluent quality, legislative compliance and operational cost.

In order to develop control strategies suitable for real life application, a flexible and transferable emission estimation model is required. Calibration is also important to ensure the validity of results, but existing models are poorly calibrated with respect to GHG emissions (if at all) and collecting sufficient data, particularly from indirect sources, is likely to be challenging.

A detailed assessment of GHG emissions would require a comprehensive model, incorporating existing methodologies for estimation of CH₄, CO₂ and N₂O emissions and sources currently omitted, to enable the relative significance of each source to be determined. However despite past investigations, there is currently a lack of reliable estimation techniques for emissions from some sources, including stripping of CH₄ formed in the sewer network and CH₄ formed under unintentionally anaerobic conditions.

In order to assess the suitability of control strategies, dynamic modelling is required and calculation of emissions must be carried out using an appropriate method. Existing models use a range of empirical and theoretical formulae for calculation of emissions and, whilst empirical formulae may be appropriate in some cases, methods with a scientific basis should be used for all sources of emissions within the wastewater treatment plant in order to ensure that the effects of control strategies are reflected in the results.

Calculation of the energy requirement and associated indirect emissions could be improved by the use of a more detailed methodology, taking into account plant specific data, the design operating point of electrical equipment and relevant efficiency curves.

Dynamic modelling of N₂O emissions poses a particular challenge; emissions resulting from nitrification and denitrification in sludge treatment and nitrogen conversion in the digester effluent, for example, were only modelled by Préndez and Lara-González (2008) and the method utilised formulae based on activity data and empirical emission factors. Keller and Hartley (2003) stated that N₂O emissions are not generally found in any significant quantity and are unlikely to contribute significantly to overall GHG emissions – however given that N₂O has a GWP 310 times greater than that of CO₂ (Defra, 2011), even low emissions would have a considerable effect and Kampschreur et al. (2009) argued that N₂O emitted during wastewater treatment could significantly add to the carbon footprint. There have been recent investigations into the factors influencing N₂O emissions (Kampschreur et al., 2009; Foley et al., 2010; Rassamee et al., 2011), and it has been shown that N₂O generation is affected by process conditions such as DO concentration in the nitrification stage and COD/N ratio in the denitrification stage; however there is no consensus on a method which can be used to estimate emissions with any degree of certainty.

More detailed emission models for individual WWTP components exist, but would require incorporating into a model with wider scope to provide a comprehensive estimation of emissions. Ni et al. (2011), for example, developed a pseudo-mechanistic model to describe the production and consumption of N₂O during activated sludge nitrification and denitrification. This model has been tested using experimental data and, if combined with other models, could provide a flexible means of calculating N₂O emissions from the activated sludge unit. A potential disadvantage of combining detailed component models, however, is the increase in the overall model complexity and resultant increase in computational demand. To ensure suitability for multiple simulation runs and control strategy optimisation, it might be necessary to simplify the model following identification of the most important sources of GHG emissions using sensitivity analysis.

CONCLUSIONS

Existing models for the assessment of GHG emissions from wastewater treatment differ vastly in both their choice of sources for inclusion and their estimation methodologies. None offer a comprehensive calculation of direct and indirect emissions and there are some potentially significant sources omitted from all. Challenges are posed by the need to calibrate models and to include emissions for which there are currently no reliable estimation methodologies.

It is thought that optimisation of control strategies could be used to reduce GHG emissions and contribute carbon reduction requirements whilst maintaining treatment standards. This would, however, require a model suitable for dynamic simulation, which is based upon theoretical relationships and would reflect the effects of changing operational conditions. Additional problems may be encountered when increasing the model detail and accuracy, due to the effect of increased computational demand on the simulation run time, particularly if optimisation is to be carried out.

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Identifying key sources of uncertainty in the modelling of greenhouse gas emissions from wastewater treatment

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Identifying sensitive sources and key control handles for the reduction of greenhouse gas emissions from wastewater treatment

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Multi-objective optimisation of wastewater treatment plant control to reduce greenhouse gas emissions

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Cost-efficient control of wastewater treatment plants to reduce greenhouse gas emissions

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Abstract: This research investigates the potential of improved wastewater treatment plant control for the cost-efficient reduction of greenhouse gas (GHG) emissions, providing a detailed exploration of the decision variable search space. Key operational parameters identified using global sensitivity analysis are sampled to provide sets of values for testing in two pre-defined control strategies. It is shown that significant reductions in emissions and costs can be realized by improved selection of parameter values. The importance of considering GHGs when selecting a control strategy is also highlighted, as the two strategies tested are shown to produce effluent of a similar quality but with significantly different emissions and operating costs.

Keywords: control; global sensitivity analysis; greenhouse gas; operation; wastewater treatment

Introduction

Global warming is an internationally recognised problem and the significance of greenhouse gas (GHG) emissions resulting from wastewater treatment processes has been highlighted in numerous studies (e.g. Rothausen and Conway 2011). Water companies are tasked with reducing their GHG emissions to assist in reaching national targets, yet they must remain economically viable and ensure adequate treatment standards are maintained.

Appropriate wastewater treatment plant (WWTP) operation can contribute greatly to the reduction of GHG emissions (Gori et al. 2011) and it has been shown that significant emission reductions can be realized by the implementation of automatic control (Flores-Alsina et al. 2011). Previous studies (Flores-Alsina et al. 2014, Guo et al. 2012b) have explored the effects of implementing a selection of different control strategies and of using different setpoints; however, conclusions drawn regarding WWTP control and performance are based on only a small number of modelled scenarios. A thorough investigation into the benefits achievable and required trade-offs is therefore required.

Multi-objective optimisation has been used to obtain a clearer picture of the trade-offs between GHG emissions, operational costs and effluent quality (Sweetapple et al. 2014). However, the results cannot be used to prescribe a specific control strategy that will provide a cost efficient reduction of GHG emissions, due to the use of a short simulation period and the potential for reduced performance when evaluated over a full year.

The objective of this work is to investigate the potential of improved control strategy design and parameterisation for the reduction of GHG emissions from WWTPs, taking into account the need to produce an acceptable effluent quality whilst remaining cost efficient and considering long term performance. Global optimisation of control strategies based on dynamic performance over an extended period is challenging due to the high computational demand of mechanistic WWTP models and large number of model evaluations required. In this study, therefore, two control strategies are considered and operational parameters to which GHG emissions,

operational costs and effluent quality are found to be most sensitive are sampled using the factorial sampling design approach to provide a search of the decision variable space.

Material and Methods

Wastewater treatment plant model

Wastewater treatment processes are simulated in BSM2-e (Sweetapple et al. 2013), a version of the Benchmark Simulation Model No. 2 (BSM2) (Jeppsson et al. 2007) modified for modelling of dynamic GHG emissions. The plant consists of a primary clarifier, five activated sludge reactors, a secondary settler, a sludge thickener, an anaerobic digester and a dewatering unit. Simulations are carried out as in BSM2, using 200 days of constant influent to allow the model to reach steady state then 609 days of dynamic influent, of which the last 364 are used for evaluation.

Sources of GHG emissions modelled include: aerobic substrate utilisation, biomass decay and denitrification in the activated sludge reactors, leakage and combustion of biogas from the anaerobic digester, stripping of methane (CH_4) from solution in the dewatering unit, generation of energy imported, manufacture of chemicals, offsite degradation of effluent, and transport and offsite degradation of sludge. Nitrous oxide (N_2O) emissions associated with nitrification are omitted due to a lack of consensus on suitable modelling techniques (models exist but have been found unable to accurately and consistently reproduce experimental data (Sperandio et al. 2014)). It is recommended that future work investigate the impact of control strategies developed in this study on such emissions, since the net impact on emissions may be less desirable than anticipated.

Emissions are reported in units of $\text{kg CO}_2\text{e/m}^3$ treated wastewater, using global warming potentials of 21 and 310 for CH_4 and N_2O respectively (IPCC 1996). Operational costs and effluent quality are assessed using an operational cost index (OCI) and effluent quality index (EQI) respectively, as defined by Jeppsson et al. (2007), and compliance is assessed with regard to the Urban Waste Water Treatment Directive requirements (European Union 1991). It must be noted that the results obtained from this model are not directly comparable with those from BSM2 due to alteration of the activated sludge model to include four-step denitrification.

Control strategies

Two different arrangements of sensors, controllers and actuators providing dissolved oxygen (DO) control are investigated, since it is known that DO control affects both operational costs (due to the impact on energy consumption (e.g. Åmand and Carlsson 2012)) and GHG emissions (e.g. Aboobakar et al. 2013). Sensitivity analysis has also shown aeration intensities in the aerobic activated sludge reactors to be key control handles for the reduction of GHG emissions, operational costs and effluent pollutant loadings (Sweetapple et al. in press).

Firstly, the BSM2 default closed loop (DCL) control strategy (Nopens et al. 2010) is implemented; and secondly, one in which the DO spatial distribution is controlled using three independent control loops (3-DO control strategy). Both are illustrated in Figure 1. The BSM2 DCL control strategy with default parameter values (Nopens et al. 2010) represents the base case. The 3-DO control strategy has previously been shown to provide an acceptable effluent quality at an acceptable cost (Vanrolleghem and Gillot 2002) and Guo et al. (2012a) found this strategy to provide the greatest

reduction in N_2O emissions. Given that N_2O is a significant contributor to total GHG emissions from wastewater treatment and the source with greatest potential for improvement (Sweetapple et al. in press), it is thought that this control strategy may provide cost-efficient reduction of emissions. Provisionally, a setpoint of $1 \text{ g O}_2/\text{m}^3$ and offset of 200 d^{-1} (Vanrolleghem and Gillot 2002) is set for every controller in this strategy.

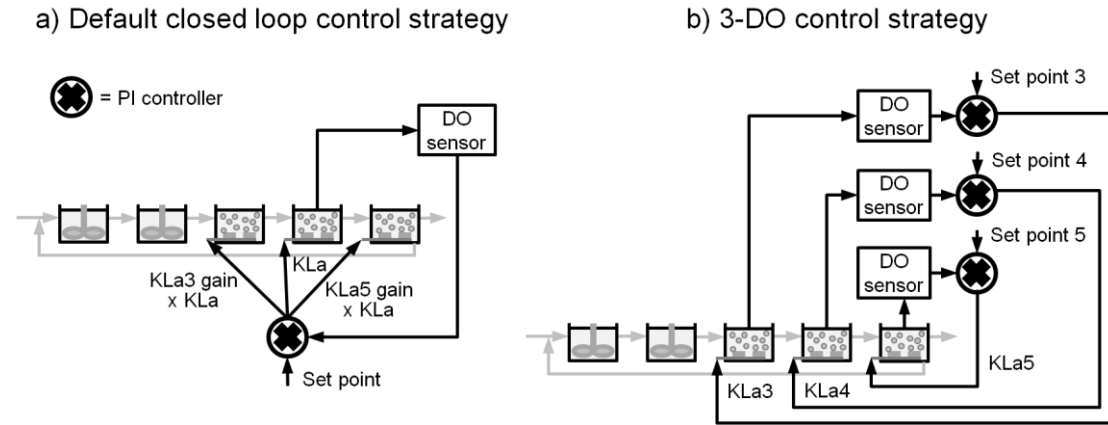


Figure 1 Control of the activated sludge unit in: a) the DCL control strategy; and b) the 3-DO control strategy.

Selection of sensitive control handles for further adjustment in this study is based on the results of global sensitivity analysis (GSA) using Sobol's method (Sobol 2001), which enables identification of significant individual and interaction effects (Sweetapple et al. in press) as shown in Figure 2.

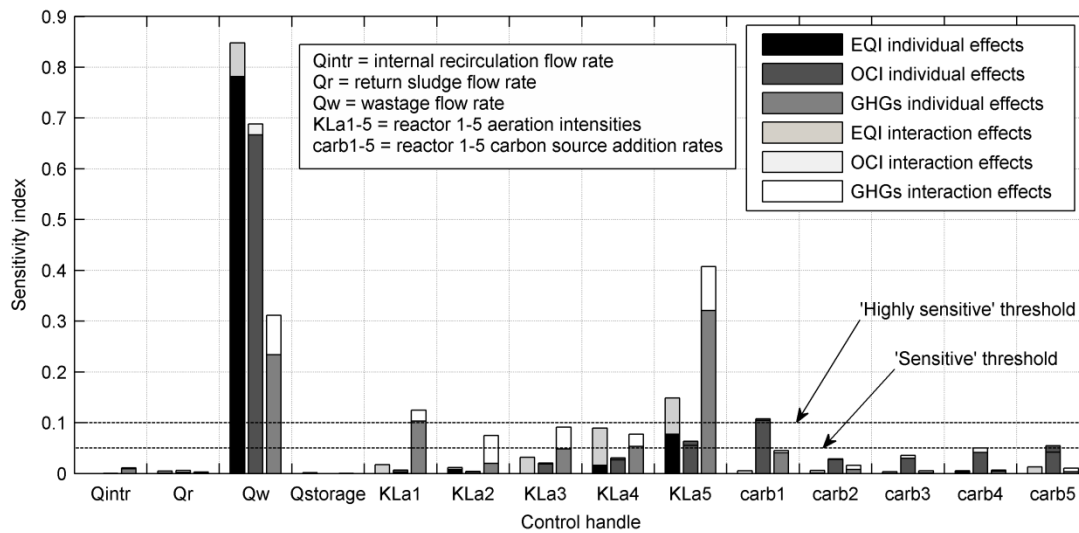


Figure 2 Sensitivity indices for WWTP operational parameters, calculated using Sobol's method, based on EQI, OCI and GHG emissions. Based on results of Sweetapple et al. (in press).

GHG emissions, OCI and EQI are all shown to be highly sensitive to wastage flow rate (Q_w) and Flores-Alsina et al. (2011) has shown significant reduction in GHG emissions to be achievable by adjustment of Q_w to change the sludge retention time (SRT). As WWTPs are subject to seasonal effects, optimal controller setpoints differ throughout the year (Stare et al. 2007) and different wastage flow rates may be implemented in order to maintain sufficient biomass in the system during winter months (e.g. Flores-Alsina et al. 2011). In this research, it is decided to implement

three different wastage rates (with values to be decided) in both control strategies throughout the year, dependent on temperature: $Q_{w_{low}}$ (when $t \leq 13.2^{\circ}\text{C}$), $Q_{w_{medium}}$ (when $13.2^{\circ}\text{C} < t \leq 16.8^{\circ}\text{C}$) and $Q_{w_{high}}$ (when $t > 16.8^{\circ}\text{C}$). Limits are set so as to provide three equal width bands, based on the observed annual temperature range.

Decision variable sampling

Factorial sampling is selected as it can provide good coverage of the search space within a relatively small number of simulations; Monte Carlo sampling, despite providing greater coverage, is not suitable due to the time taken for each model evaluation.

A 10-level factorial sampling design is used to generate a set of values for $Q_{w_{low}}$, $Q_{w_{medium}}$ and $Q_{w_{high}}$ within the range 93.5 to 506.5 m³/d for the DCL control strategy. This contains 1,000 samples, reduced to 220 when instances in which $Q_{w_{low}} > Q_{w_{medium}}$ or $Q_{w_{medium}} > Q_{w_{high}}$ are removed. Samples evaluated in the 3-DO control strategy are restricted to 84 in which $Q_{w_{low}} > 139.5 \text{ m}^3$, since these were consistently found to produce a compliant effluent in the DCL control strategy.

Given that the control handle KLa_5 is also shown to be key for the reduction of GHG emissions and is classified as sensitive or highly sensitive based on all three performance indicators (Sweetapple et al. in press), the DO set point for reactor 5 in the 3-DO control strategy is also considered as a decision variable. This is sampled within the range 0.5 to 2.5 g O₂/m³ using 5-level factorial sampling for each combination of wastage flow rates.

Results and Discussion

Wastage flow rate adjustment

Performance of control strategies with adjusted wastage flow rates which produce a compliant effluent is shown in Figure 3. It is observed that implementation of different combinations of Q_w values can enable a reduction of both GHG emissions and OCI simultaneously whilst maintaining compliance in both control strategies.

In the DCL control strategy, GHG emissions can be reduced by up to 6.0% with respect to the base case whilst also reducing the OCI by 2.3%. The lowest emission solution uses a constant wastage flow rate of 185.3 m³/d – corresponding to a significantly longer SRT than in the base case (28 days mean compared with 15 days). The predominant source of reduction in operating costs is the reduction of sludge produced for disposal, not reduction in pumping costs as may be expected. Energy costs actually increase due to increased aeration requirements to maintain the specified setpoint. Reduction in GHG emissions associated with a reduction in energy required for pumping is also negligible (0.1% contribution). Change in N₂O emissions from the activated sludge reactors provide 131% of the net reduction in emissions whilst non-N₂O emissions from the activated sludge reactors provide -61% (i.e. they increase). This supports the observation of Flores-Alsina et al. (2011) that a high SRT increases direct non-N₂O emissions from the bioreactor and indirect emissions resulting from electricity use.

The reduction in GHG emissions and OCI achievable by adjustment of wastage flow rate in the default open loop control strategy also corresponds with an increase in EQI (although all solutions presented remain compliant, and in some instances the

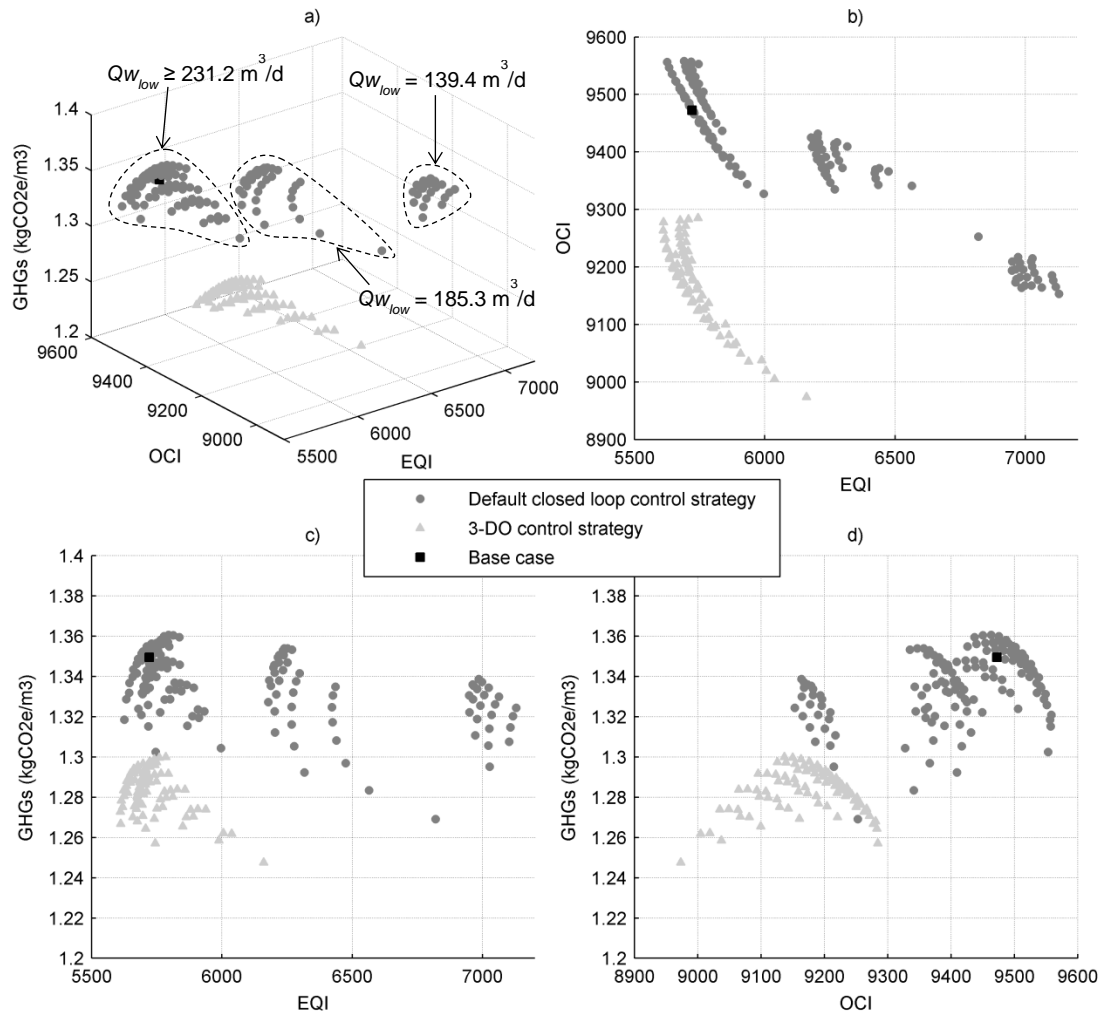


Figure 3 WWTP performance with adjusted control strategy wastage flow rates (compliant solutions only).

impact on effluent quality is minor); all solutions which reduce the EQI increase operational costs. GHG emissions and EQI can be reduced simultaneously through improved control of wastage flow rates, but this is at the expense of OCI.

Solutions in the 3-DO control strategy have significantly lower GHG emissions and operating costs than those with a comparable effluent quality in the DCL control strategy. This highlights the importance of evaluating a range of alternative control options and suggests that, of the two studied, the 3-DO control strategy offers superior performance with regard to GHG emissions, operational costs and effluent quality. It also supports recommendation that implementation of the 3-DO control strategy would be economically wise (Vanrolleghem and Gillot 2002).

Using the 3-DO control strategy, an equivalent effluent quality to that of the base case can be maintained whilst reducing GHG emissions by 6.3% and also cutting operational costs by 2.0%, by implementing wastage flow rates of 231.2, 231.2 and 277.1 m³/d for $Q_{w_{low}}$, $Q_{w_{medium}}$ and $Q_{w_{high}}$ respectively. This solution provides a mean SRT of 22 days – again, significantly greater than that of the base case.

It may be thought that selection of a control strategy in which energy recovery from biogas combustion is reduced would be undesirable in terms of both operational costs and GHG emissions. This specific solution, however, exhibits a net decrease in both

OCI and GHG emissions despite enabling less energy recovery than the base case control strategy: the increase in operational costs as a result of reduced energy recovery is less than the cost saving resulting from reduced sludge production, and the total indirect emissions resulting from net energy import decrease due to the reduction in energy required for pumping and aeration.

It is also found that implementing solutions providing a shorter SRT can be of benefit with regard to cost and emissions: the solution providing the greatest emission reduction (7.6%) in the 3-DO control strategy has a constant Q_w value of 506 m³/d (upper limit of range tested) and a mean SRT of 11 days and provides a reduction in both N₂O and non-N₂O emissions from the activated sludge unit. However, this also causes a 7.7% increase in EQI.

These contrasting combinations of Q_w values shown to provide a reduction in net GHGs with no additional operational costs demonstrate that an emission reduction is achievable with different approaches to SRT control, each of which affects different sources of emissions. Given the trade-off in EQI observed with a high wastage flow rates, however, it is suggested that a high SRT solution may be preferable. Furthermore, emissions not included in this study are likely to be significant in low SRT solutions: for example, N₂O emissions from biological hydroxylamine oxidation occur mainly at high NH₄⁺ and low NO₂⁻ concentrations (Wunderlin et al. 2012), which are likely to be present with a low SRT.

Dissolved oxygen setpoint adjustment

Figure 4 shows that adjustment of DO concentrations in the final aerobic reactor (by manipulation of the DO setpoint) in addition to Q_w enables the development of solutions which further improve upon the base case GHG emissions and OCI whilst having negligible impact on effluent quality. Conversely, selection of too high a setpoint is found to increase GHG emissions and OCI.

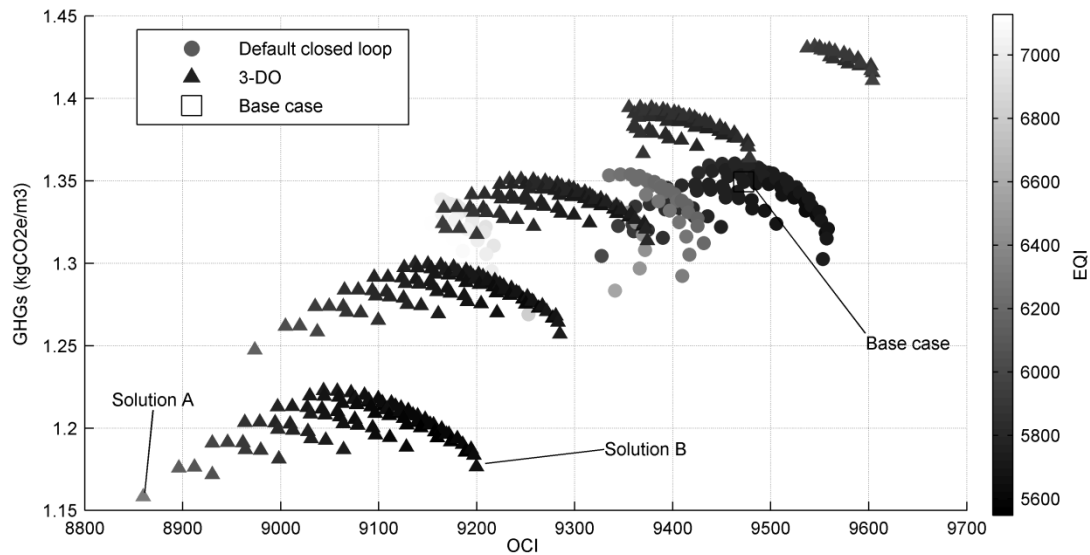


Figure 4 WWTP performance with adjusted reactor 5 DO setpoint in the 3-DO control strategy and adjusted wastage flow rates in both (compliant solutions only); colour denotes EQI, with a darker shade representing a better quality effluent.

The cluster of solutions found to perform best with regard to OCI and GHG emissions all have a reduced DO setpoint of 0.5 g O₂/m³. To enable analysis of the effects of Q_w adjustments on different contributors to operational costs and GHG

emissions, two solutions in this cluster are compared in Table 1: Solution A provides the lowest GHG emissions and OCI but at the expense of effluent quality, solution B provides a smaller (but still significant) emission and cost reduction with regard to the base case but with no loss in effluent quality.

Table 1 Comparison of solutions, with percentage contribution of component change to total change in performance indicator in brackets. Only GHG and OCI components of interest are shown. Components worsened with respect to the base case are highlighted.

Solution		Base case	A	B
Aeration control		DCL	3-DO	3-DO
Mean SRT (days)		15.5	11.4	23.2
GHG components (kg CO ₂ e/m ³)	N ₂ O from activated sludge	0.50	0.34 (83%)	0.31 (111%)
	Non-N ₂ O from activated sludge	0.39	0.35 (20%)	0.43 (-24%)
	Pumping energy	0.01	0.01 (0%)	0.01 (0%)
	Aeration energy	0.05	0.04 (4%)	0.05 (1%)
	Sludge transportation and degradation	0.05	0.06 (-1%)	0.05 (2%)
OCI components (-)	Energy use	5560	4975 (95%)	5369 (70%)
	Energy recovery	-6425	-6693 (44)	-6089 (-123%)
	Sludge for disposal	7938	8178 (-39%)	7519 (153%)
Performance indicators	Total GHGs (kg CO ₂ e/m ³)	1.35	1.16	1.18
	OCI	9472	8860	9200
	EQI	5722	6298	5670

As with the DCL control strategy, a high SRT solution results in an increase in non-N₂O emissions from the activated sludge but this is offset by the decrease in N₂O emissions to give a net reduction.

In solution A, the cost reduction is achieved primarily through a reduction in energy use and an increase in energy recovery. Solution B, however, provides significantly less energy recovery than the base case yet still offers a reduction in overall operational costs and GHG emissions and a greatly improved effluent quality. This again suggests that solutions providing the greatest energy recovery from biogas production may not necessarily be the most desirable in terms of net benefits.

Conclusions

This study has investigated WWTP performance with regard to GHG emissions, operational costs and effluent quality under two different control strategies and with a range of wastage flow rates and DO setpoints. It is found that independent control of aeration in each aerated activated sludge reactor, in particular when using a low reactor 5 DO setpoint, enables significant reduction in both GHG emissions and operational costs whilst maintaining a high effluent quality. However, in both control strategies analysed, significant improvements can be achieved through better control of wastage flow rates alone.

The results emphasise the importance of considering the effects of emission reduction measures on emissions from a range of different sources rather than focussing on just one high priority source. Increasing the SRT, for example, can result in emission and cost reduction but direct non-N₂O emissions are increased. Furthermore, it is suggested that developing control strategies to provide the greatest possible energy recovery may not always be necessary (or desirable) with regard to reducing GHG emissions and operational costs, since the effects of reduced energy recovery can be offset by the reduction in cost and emissions associated with sludge disposal, and a greater effluent quality may be achieved.

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